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Computational Quantum Field Theory

10.1 Introduction

The Computational Physics Group performs basic research into classical and quantum statistical physics with special emphasis on phase transitions and critical phenomena. In the centre of interest are the physics of spin glasses, diluted magnets and other materials with quenched, random disorder, soft condensed matter physics with focus on fluctuating paths and interfaces, biologically motivated problems such as protein folding, aggregation and adsorption as well as related properties of homopolymers, and the intriguing physics of low-dimensional quantum spin systems. Our investigations of a geometrical approach to the statistical physics of topological defects with applications to superconductors and superfluids and research into fluctuating geometries with applications to quantum gravity, e.g., dynamical triangulations, build on the recently concluded European Research Training Network (RTN) "ENRAGE": *Random Geometry and Random Matrices: From Quantum Gravity to Econophysics*, a collaboration of 13 teams throughout Europe. Moreover, within a bi-national Institute Partnership initiated by a research grant of the Alexander von Humboldt Foundation the statistical mechanics of complex networks is studied in collaboration with our partner university in Krakow, Poland.

The methodology is a combination of analytical and numerical techniques. The numerical tools are currently mainly Monte Carlo computer simulations and high-temperature series expansions. The computational approach to theoretical physics is expected to gain more and more importance with the future advances of computer technology, and is likely to become the third cornerstone of physics besides experiment and analytical theory as sketched in Fig. 10.1. Already now it can help to bridge the gap between experiments and the often necessarily approximate calculations of analytical work.

To achieve the desired high efficiency of the numerical studies we develop new algorithms, and to guarantee the flexibility required by basic research all computer codes are implemented by ourselves. The technical tools are Fortran, C, and C++ programs running under Unix or Linux operating systems and computer algebra using Maple or Mathematica. The software is developed and tested at the Institute on a cluster of PCs and workstations, where also most of the numerical analyses are performed.

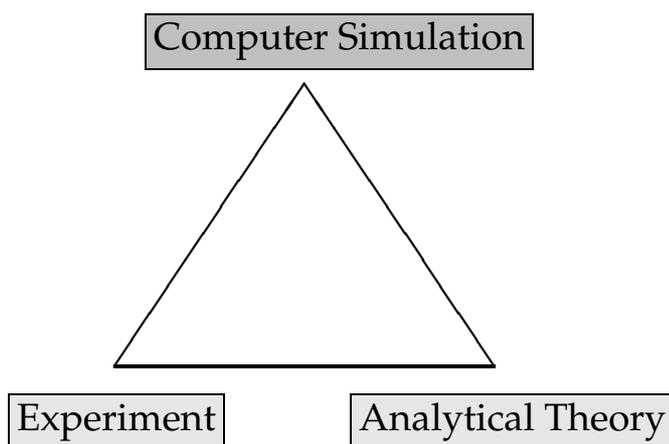


Figure 10.1: Sketch of the relationship between theory, experiment and computer simulation.

Currently we are also exploring the possibilities of the rapidly developing graphics card computing, that is computer simulations on graphics processing units (GPUs) with many cores. Large-scale simulations requiring vast amounts of computer time are carried out at the Institute on quite powerful compute servers, at the parallel computers of the University computing center, and, upon successful grant application at the national supercomputing centres in Jülich, Stuttgart and München on parallel supercomputers. This hierarchy of various platforms gives good training opportunities for the students and offers promising job perspectives in many different fields for their future career.

Within the University, our research activities are closely integrated into the Graduate School “BuildMoNa”: Leipzig School of Natural Sciences – *Building with Molecules and Nano-objects* funded by the German Research Foundation (DFG) within the German Excellence Initiative and the international DFH-UFA Graduate School *Statistical Physics of Complex Systems* with Nancy Université, France, supported by the Deutsch-Französische Hochschule. For the latter we submitted in 2010 a successful extension proposal, securing enhanced funding for the period 2011–2013 and now incorporating also Coventry University in England as an associated partner. The two Graduate Schools are both “Classes” of the Research Academy Leipzig (RALeipzig), providing the organizational frame for hosting visiting students and senior scientists, offering language courses, organizing childcare and for many other practical matters. At the post-graduate level our research projects are embedded into the “Sächsische DFG-Forschergruppe” FOR877 *From Local Constraints to Macroscopic Transport*, which also has been successfully extended in 2010 for the period 2011–2014, the Sonderforschungsbereich/Transregio SFB/TRR 102 *Polymers under Multiple Constraints: Restricted and Controlled Molecular Order and Mobility* together with Halle University, which started operation in July 2011, and the International Max Planck Research School (IMPRS) *Mathematics in the Sciences*. Our group also actively contributes to two of the top level research areas (“Profilbildende Forschungsbereiche (PbF)”) and the Centre for Theoretical Sciences (NTZ) of the University. Beside “BuildMoNa” the latter structures are particularly instrumental for our cooperations with research groups in experimental physics and biochemistry on the one hand and with mathematics and computer

science on the other.

On an international scale, our research projects are carried out in a wide net of collaborations funded by the German Academic Exchange Service (DAAD) and the Alexander von Humboldt Foundation through the Institute Partnership with the Jagiellonian University in Krakow, Poland, as well as their Fellowship Programmes, and in part initiated by the European Research Training Network "ENRAGE". Since June 2011 our group is hosting Professor Handan Arkin-Olgar from Ankara University in Turkey who was awarded an Alexander von Humboldt Fellowship for Experienced Researchers. Further close contacts and collaborations are established with research groups in Armenia, Austria, China, France, Great Britain, Israel, Italy, Japan, Poland, Russia, Spain, Sweden, Taiwan, Turkey, Ukraine, and the United States. These contacts are refreshed and furthered through topical Workshops and Tutorials and our International Workshop series *CompPhys: New Developments in Computational Physics*, taking annually place at the end of November just before the first advent weekend.

Wolfhard Janke

10.2 How Grafting of a Single Polymer Influences its Statistical Properties near an Attractive Substrate

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There is a significant difference in the conformational behaviour of a polymer grafted, i.e. firmly attached at one end, to an attractive substrate compared to one that can move freely within a certain distance to that substrate [1]. Especially at the adsorption transition, we expected such differences after a microcanonical analysis of the nongrafted polymer revealed first-order like signals for short extended conformations that get more pronounced with increasing translational entropy of desorbed conformations [2, 3]. To systematically compare the two cases, a combined canonical and microcanonical analysis was performed for a wide range of surface attraction strengths ϵ_s and temperature T [4]. This way not only the adsorption transition, but also the collapse and the freezing transition of an individual self-interacting polymer in solution were covered.

The model is a simple bead-stick model with 12-6 Lennard-Jones (LJ) interaction between nonbonded monomers, a weak bending stiffness and an attraction to a flat substrate that is proportional to a parameter ϵ_s . This surface attraction is a 9-3 LJ potential obtained by integrating the 12-6 LJ potential over a half space and, e.g., $\epsilon_s = 5$ roughly gives a surface attraction that exceeds the monomer-monomer attraction by a factor of five. This model is once considered in a box within which it can move freely and once with one end grafted to the substrate. All simulations were performed with the parallel tempering Monte Carlo method that allowed to highly parallelize the simulation and obtain good statistics over the whole energy range.

It turned out, that qualitative differences really only occur at the adsorption transition. Here, however, four cases need to be differentiated for finite chains: (1) the adsorption of extended nongrafted polymers, (2) the adsorption of extended grafted

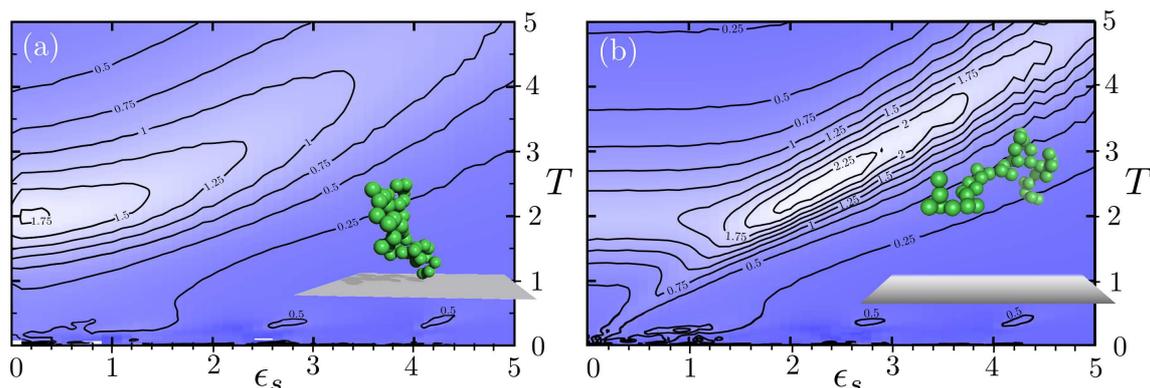


Figure 10.2: Fluctuation of the tensor component of the radius of gyration perpendicular to the substrate $d\langle R_{\text{gyr},\perp}^2\rangle/dT$ for (a) the grafted and (b) the free polymer as a contour plot versus surface attraction strength ϵ_s and temperature T .

polymers, (3) the adsorption of globular nongrafted polymers and (4) the adsorption of globular grafted polymers. Only in the first case, the microcanonical entropy, which is proportional to the logarithm of the density of states, gets convex such that the adsorption transition is first-order-like here with a dynamic phase coexistence. In the cases (2) and (3) a continuous adsorption is observed already for short chains, while in case (4) the adsorption signals get reduced significantly and only the weaker wetting transition is left.

How this is for example reflected in the temperature derivative of the canonical expectation value of the tensor component of the radius of gyration perpendicular to the substrate is visualized in Fig. 10.2. While for the nongrafted polymer a maximum over the whole diagonal $T_{\text{ads}} \propto \epsilon_s$ is visible, this signal is strongly weakened for extended grafted conformations ($\epsilon_s \gtrsim 1.9$, $T \gtrsim 2$) and even disappears for globular grafted conformations ($\epsilon_s \lesssim 1.9$, $T \lesssim 2$). For grafted chains, in this observable only the collapse transition at $T \approx 2$ is signaled for low ϵ_s values.

It is among others this necessary distinction between the adsorption of globular and extended conformations that demonstrates that it is not just the difference in translational, but also in conformational entropy that gives rise to the differences. This has been carefully described and explained in Ref. [4].

- [1] M. Möddel et al.: J. Phys. Chem. B **113**, 3314 (2009)
- [2] M. Möddel et al.: Phys. Chem. Chem. Phys. **12**, 11548 (2010)
- [3] M. Möddel et al.: Comput. Phys. Commun. **182**, 1961 (2011)
- [4] M. Möddel et al.: Macromolecules **44**, 9013 (2011)

10.3 Thermodynamics of Polymer Adsorption to a Flexible Membrane

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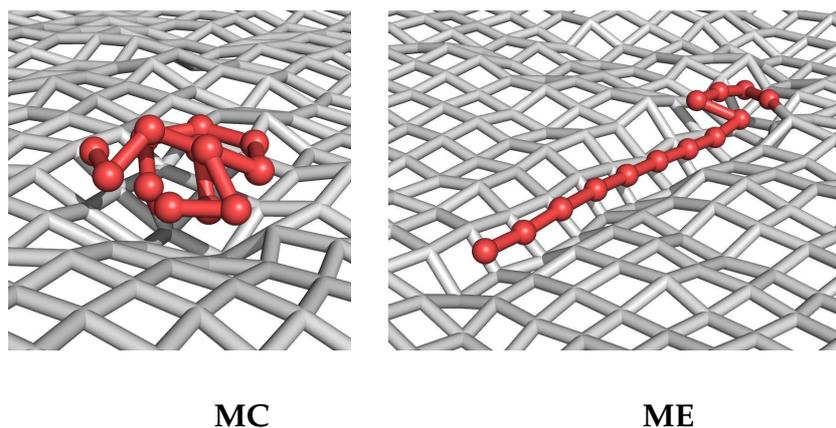


Figure 10.3: Embedded compact (MC) and expanded (ME) conformations exhibited by a polymer grafted to a flexible membrane at low temperatures and strong polymer-membrane attraction.

The interaction of macromolecules with cell membranes is essential for almost all biological processes. Membrane proteins like glycoproteins and transmembrane proteins govern the exchange of signals, small molecules, and ions between the intra- and extra-cellular solvent. Membrane embedded receptors are specific for the binding of ligands. The conformational changes caused by the binding process can, e.g., trigger cellular motion, drug delivery, or enzymatic catalysis.

It is therefore an important problem to investigate the conformational behaviour of a polymer interacting with a *flexible, fluctuating* substrate such as a membrane under thermal conditions. So far much work has been dedicated to the identification of structural transitions polymers and peptides experience when adsorbing to *solid* substrates [1–4]. In this project we extend these studies by considering a simple coarse-grained off-lattice model system consisting of a polymer grafted to a fluctuating substrate and performing extensive generalized-ensemble Monte Carlo computer simulations [5]. Adjacent monomers of the polymer are tied together by a finitely extensible nonlinear elastic (FENE) potential and all monomers interact pairwise via a standard 12–6 Lennard-Jones (LJ) potential. The fluctuating substrate is modeled by a tethered membrane with the individual building segments (nodes) again tied together by a FENE potential to form a 2D surface with $L_x \times L_y$ nodes in total. Finally, the interaction between the polymer, which is anchored at the membrane center, and the membrane is modeled by another LJ potential between all pairs of monomers and membrane nodes.

By means of extensive parallel tempering Monte Carlo simulations we have shown that the system exhibits a rich phase behaviour ranging from highly ordered, compact to extended random coil structures and from desorbed to completely adsorbed or even partially incorporated conformations, cf. Fig. 10.3. These findings are summarized in the pseudophase diagram shown in Fig. 10.4 indicating the predominant class of conformations as a function of the external parameters polymer-membrane interaction strength and temperature. By comparison with adsorption to a stiff membrane surface it is shown that the flexibility of the membrane gives rise to qualitatively new behaviour. At low temperatures, we found the membrane adapting its structure such that it partially incorporates the polymer. This leads to the “embedded compact” (MC), oblate shaped and the “embedded expanded” (ME), almost linearly stretched conformations

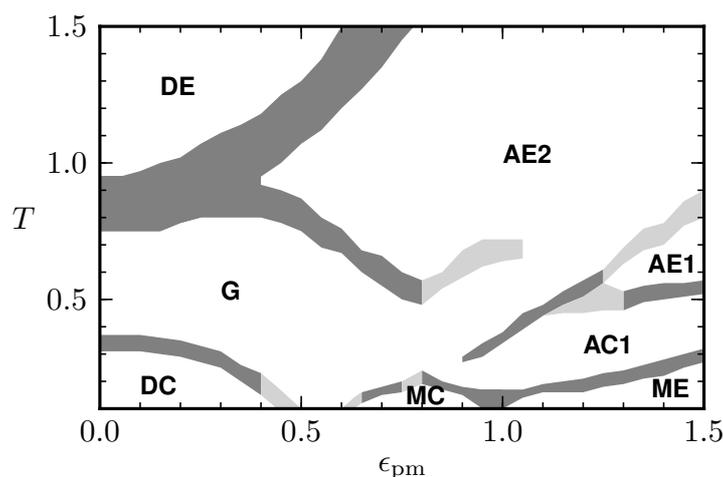


Figure 10.4: Phase diagram of a polymer grafted to a fluctuating membrane parametrized by polymer-membrane attraction strength ϵ_{pm} and temperature T . The letter code stands for DE = desorbed expanded, G = globular, DC = desorbed compact, AE = adsorbed expanded, and AC = adsorbed compact. Representative conformations of the embedded compact (MC) and expanded (ME) phases are shown in Fig. 10.3.

shown in Fig. 10.3, which both most clearly reflect the influence of the back-reaction between polymer and membrane fluctuations.

- [1] M. Bachmann, W. Janke: Phys. Rev. Lett. **95**, 058102 (2005); Phys. Rev. E **73**, 041802 (2006); Phys. Rev. E **73**, 020901(R) (2006); Phys. Part. Nucl. Lett. **5**, 243 (2008)
- [2] M. Möddel et al.: J. Phys. Chem. B **113**, 3314 (2009)
- [3] M. Möddel et al.: Phys. Chem. Chem. Phys. **12**, 11548 (2010); Comput. Phys. Commun. **182**, 1961 (2011)
- [4] M. Möddel et al.: Macromolecules **44**, 9013 (2011)
- [5] S. Karalus et al.: Phys. Rev. E **84**, 031803 (2011)

10.4 Polymer Adsorption to a Fractal Substrate

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The conformational statistics of polymers interacting with substrates is a subject of growing interest in polymer science. It plays an important role both in technology (adhesion, stabilization of colloidal dispersions) and biological physics (proteins adsorption on membranes) [1]. Particularly interesting is the case of an attractive substrate, where below a critical temperature T_A a second-order phase transition into an adsorbed state takes place. As order parameter one considers the fraction of the average number of monomers N_s adsorbed to the surface and the total length N of the polymer chain, obeying for long chains the scaling law $\langle N_s \rangle / N \sim N^{\phi_s - 1}$ where ϕ_s is the surface

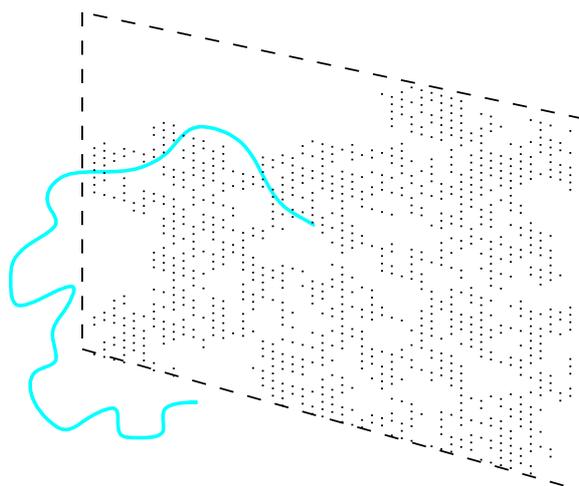


Figure 10.5: Sketch of a polymer chain grafted to an attractive “sieve” formed by a percolation cluster.

crossover exponent [2]. Most naturally occurring substrates are rough and energetically (or structurally) inhomogeneous, and, in fact, are often of fractal nature. In the language of lattice models, where polymers can be represented by self-avoiding random walks (SAWs) [3], such surfaces can be modeled as a two-dimensional regular lattice with different types of randomly distributed defects. Fractal properties emerge at the percolation threshold where a spanning percolation cluster of attractive sites with fractal dimension $d_s^{p_c} = 91/49 \approx 1.89 < 2$ appears [4], cf. Fig. 10.5.

We have studied this problem with the help of the pruned-enriched Rosenbluth method (PERM) [5] for simulating the polymer chains. We examined the behaviour of the components of the radius of gyration $\langle R_{g\parallel}^2 \rangle$, $\langle R_{g\perp}^2 \rangle$ in directions parallel and perpendicular to the surface, and found that the critical exponent governing the scaling of the size of the polymer chain adsorbed on a fractal substrate formed by a percolation cluster is larger than that for a homogeneously attractive surface. A value $\nu_2^{p_c} = 0.772 \pm 0.006$ is obtained [6], to be compared with the compatible result $\nu_2^{p_c} = 0.782 \pm 0.003$ for the average size of a polymer strictly confined onto a two-dimensional percolating cluster [7] and $\nu_2 = 0.742 \pm 0.006 \approx 3/4$ for a plain surface [6]. Examining the peak structure of the heat capacity, we find an estimate for the surface crossover exponent $\phi_s^{p_c} = 0.425 \pm 0.009$, compared to $\phi_s = 0.509 \pm 0.009$ for the plain surface [6]. As expected, the adsorption is diminished, when the fractal dimension of the surface is smaller than that of the plain Euclidean surface due to the smaller number of contacts of monomers with attractive sites.

- [1] A.F. Xie, S. Granick: *Nature Materials* **1**, 129 (2002)
- [2] E. Eisenriegler et al.: *J. Chem. Phys.* **77**, 6296 (1982)
- [3] C. Vanderzande: *Lattice Models of Polymers* (Cambridge University Press, Cambridge (England) 1998)
- [4] S. Havlin, D. Ben Abraham: *Adv. Phys.* **36**, 155 (1987)
- [5] P. Grassberger: *Phys. Rev. E* **56**, 3682 (1997)
- [6] V. Blavatska, W. Janke: *J. Chem. Phys.* **136**, 104907 (2012)
- [7] V. Blavatska, W. Janke: *Europhys. Lett.* **82**, 66006 (2008); *J. Phys. A* **42**, 015001 (2009)

10.5 Polymer Chain Inside an Attractive Sphere Potential

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A most important class of molecules in living cells consists of various types of proteins. Their importance to biological systems cannot be overstated [1]: they catalyze and regulate the cell's activities when acting as enzymes. As is well known, proteins with globular structure fold into compact configurations in which they are biologically active. The cellular environment in which a protein folds and performs its functions is crowded with several biological molecules including lipids, carbohydrates and other proteins. An important issue is understanding the mechanism by which proteins attain their folded structure, factors that contribute to the folding and the environmental conditions that make the folding transition possible [2, 3]. Such understanding is important not only as a scientific issue but also due to debilitating diseases such as Alzheimer's and Parkinson's that are believed to be the result of accumulation of toxic protein aggregates [4]. Although the three-dimensional structure of native proteins is controlled mostly by their amino acid sequence, their transport properties and the kinetics of their folding depend on the local environment. But, whereas protein folding in dilute solutions under bulk conditions is relatively well understood, because most of experimental, theoretical and computational studies on protein folding have relied on studying proteins in the infinitely dilute limit, the more important problem of protein folding in a confined environment is not. The understanding of protein folding in confined or crowded media is one of the most challenging objectives in biologically motivated research. It is crucial to understand for a given protein what are the thermally accessible conformations, the folding pathways and controlling parameters from the environment, of which some of them have been explored in detail in Refs. [5, 6]. Also adsorption phenomena near flat surfaces within lattice and off-lattice formulations have been investigated [7, 8].

In this study [9], we performed multicanonical Monte Carlo simulations in order to determine the thermodynamic and structural properties of a polymer chain inside an attractive, unstructured sphere. The main objective of this study is to analyze the influence of the attracting sphere in terms of thermodynamical quantities when varying the attraction strength ϵ of the sphere and temperature T . All these canonical expectation values of energetic and structural quantities and their thermal fluctuations are summarized in the pseudophase diagram in the $\epsilon - T$ plane shown in Fig. 10.6.

- [1] C. Branden, J. Tooze: *Introduction to Protein Structure* (Garland Publishing, New York 1998)
- [2] C.B. Anfinsen: *Science* **181**, 223 (1973)
- [3] D.K. Klimov, D. Thirumalai: *Phys. Rev. Lett.* **76**, 4070 (1996); L. Mirny, E. Shakhnovich: *Annu. Rev. Biophys. Biomol. Struct.* **30**, 361 (2001)
- [4] M. Hayer-Hartl, A.P. Minton: *Biochemistry* **45**, 13356 (2006); D.A. Kirschner et al.: *Proc. Natl. Acad. Sci. (USA)* **83**, 503 (1986); E.H. Koo et al.: *ibid.* **96**, 9989 (1999); K.A. Conway et al.: *ibid.* **97**, 571 (2000); D.G. Lynn, S.C. Meredith: *J. Struct. Biol.* **130**, 153 (2000)

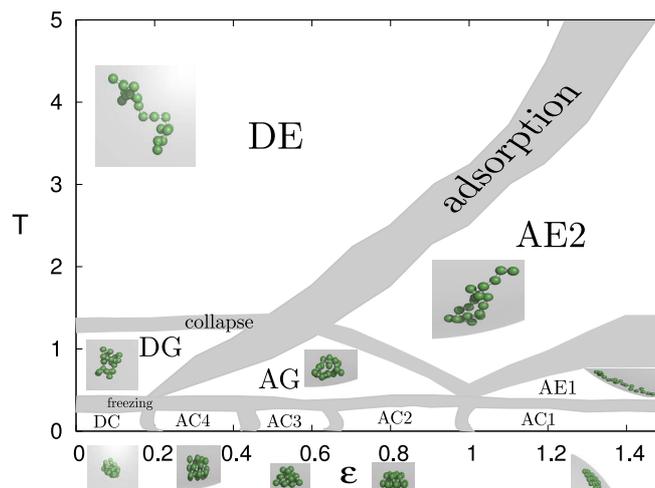


Figure 10.6: The phase diagram of the homopolymer-attractive sphere system as obtained in extensive computer simulations. The boundaries in the phase diagram separate the individual conformational phases. The band width shows the variation of the corresponding peaks of the temperature derivatives of different structural observables which are analyzed simultaneously. DE, DG, and DC denote the desorbed phases of expanded, globular and compact/crystalline conformations, respectively. AE1 stands for completely adsorbed expanded structures and AE2 for partially adsorbed expanded structures. AG reflects the adsorbed globular regime and the compact/crystalline structures occur with different topologies. These have different number of layers: AC4 – adsorbed spherically symmetric, AC3 – adsorbed three-layer structures, AC2 – adsorbed two-layer structures, and finally AC1 – adsorbed mono-layer structures.

- [5] S. Schnabel et al.: Phys. Rev. Lett. **98**, 048103 (2007); J. Chem. Phys. **126**, 105102 (2007)
- [6] H. Arkin: Phys. Rev. E **78**, 041914 (2008)
- [7] M. Bachmann, W. Janke: Phys. Rev. Lett. **95**, 058102 (2005); Phys. Rev. E **73**, 041802 (2006); Phys. Rev. E **73**, 020901(R) (2006)
- [8] C. Junghans et al.: Phys. Rev. Lett. **97**, 218103 (2006); J. Chem. Phys. **128**, 085103 (2008); M. Möddel et al.: J. Phys. Chem. B **113**, 3314 (2009); Phys. Chem. Chem. Phys. **12**, 11548 (2010); Comput. Phys. Commun. **182**, 1961 (2011); Macromolecules **44**, 9013 (2011)
- [9] H. Arkin, W. Janke: Phys. Rev. E **85**, 051802 (2012)

10.6 Thermodynamics of a Model Protein in Spherical Confinement

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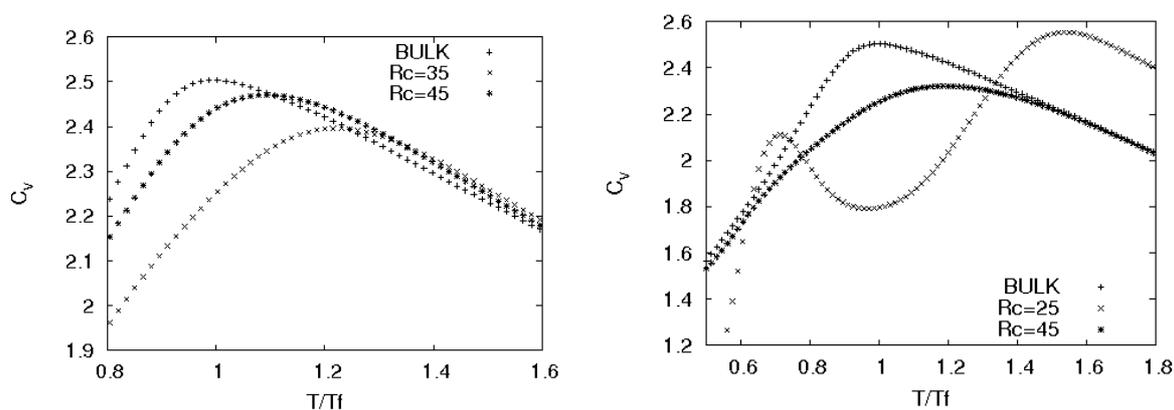


Figure 10.7: Specific heat as a function of temperature for the AB model protein $BA_6BA_4BA_2BA_2B_2$ in a spherical confinement with sphere radius R_c . The temperature T is given in units of the folding temperature T_f in the bulk. *Left:* Purely repulsive potential. *Right:* Attractive potential.

We have performed Monte Carlo computer simulations in generalized ensembles of a model protein confined in a spherical cage to investigate the dynamics of the folding mechanism [1]. The problem of whether proteins are misfolded or aggregated or, on the contrary, fold properly more promptly in spatial confinement has recently attracted much interest [2, 3]. A detailed understanding of this subject would play a key role for finding treatments to diseases caused by misfolding of proteins. Our goal is thus to analyze the thermodynamics of the folding mechanism and to investigate whether the folding mechanism is controlled or not in a confining environment. To do so we have employed exhaustive multicanonical Monte Carlo simulations by using a minimalistic AB model where hydrophobic residues are labeled by A and the polar or hydrophilic ones by B [4, 5]. Adjacent residues or monomers are connected by rigid covalent bonds. Thus, their distance is kept fixed and set to unity. The contact interaction is replaced by a distance- and residue-dependent 12 – 6 Lennard-Jones potential accounting for short-range excluded volume repulsion and long-range interaction. An additional interaction accounts for the bending energy of any pair of successive bonds. In this study, we focused on the folding of a model protein with 20 residues arranged in the sequence $BA_6BA_4BA_2BA_2B_2$.

The model protein is enclosed by a sphere of radius R_c . Apart from the steric hindrance effect, we assumed two different types of wall interactions, one with a purely repulsive wall potential and another that exhibits an attractive part close to the inner sphere wall. By monitoring the specific heat as a function of temperature, we observe in the first, purely repulsive case merely a monotonic finite-size scaling shift of the folding temperature, cf. Fig. 10.7 (left). The second case with attractive wall interaction is much more interesting since here, for small enough sphere radius R_c , the protein is first adsorbed to the (inner) surface of the sphere and in a second step the folding takes place. This is indicated by the two peaks of the specific heat for $R_c = 25$ in Fig. 10.7 (right) [6].

[1] J.A. Hubbell: *Curr. Opin. Biotechnol.* **10**, 123 (1999); S. Santosa et al.: *Nano Lett.* **2**,

- 687 (2002); S. Vauthey et al.: Proc. Natl. Acad. Sci. USA **99**, 5355 (2002)
- [2] F. Takagi et al.: Proc. Natl. Acad. Sci. USA **100**, 11367 (2003); N. Rathore et al.: Biophys. J. **90**, 1767 (2006); D. Lu et al.: Biophys. J. **90**, 3224 (2006)
- [3] S. Kumar, M.S. Li: Phys. Rep. **486**, 1 (2010)
- [4] F.H. Stillinger, T. Head-Gordon: Phys. Rev. E **52**, 2872 (1995); A. Irbäck et al.: Phys. Rev. E **58**, R5249 (1998)
- [5] M. Bachmann et al.: Phys. Rev. E **71**, 031906 (2005)
- [6] M. Bilsel et al.: *Effects of confinement on the thermodynamics of a model protein*, Ankara/Leipzig preprint (2011)

10.7 Shapes of Θ -Polymers in Crowded Media under Stretching Force

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Long flexible polymers in a good solvent form crumpled coil conformations which are perfectly described by self-avoiding random walks (SAW) on a regular lattice [1]. This regime holds at temperatures T well above the so-called Θ -point. When lowering the temperature, the effect of monomer-monomer attraction grows and the polymer radius shrinks. At $T = T_\Theta$, a crossover occurs from high-temperature SAW behaviour to the Θ -statistics. At this particular temperature, polymers in $d = 3$ dimensions behave effectively as simple random walks (RW). Below the Θ -temperature, the entropic effects, which make the polymer chain swell, are overcome by interaction energy and a collapse to the globule regime occurs. The coil-globule transition is considered to be of second order [1], in the sense that the density of an infinite globule is zero at $T = T_\Theta$ and increases continuously when further lowering the temperature.

The coil-globule transition is of interest in various respects, being deeply connected with problems like protein folding and DNA condensation. The properties of polymers in the vicinity of the Θ -point can be successfully studied on the basis of self-attracting self-avoiding walks (SASAW), where a nearest-neighbor interaction is included: an attractive energy $-\epsilon$ between two neighbour sites is introduced. When studying the folding dynamics and transport properties of proteins, an important role is played by global shape properties of a typical polymer conformation. The asymmetry of polymer shape can be characterized, e.g., by the invariant asphericity [2]

$$A_d = \frac{1}{d(d-1)} \sum_{i=1}^d \frac{(\lambda_i - \bar{\lambda})^2}{\bar{\lambda}^2} = \frac{d}{d-1} \frac{\text{Tr } \hat{\mathbf{Q}}^2}{(\text{Tr } \mathbf{Q})^2}, \quad (10.1)$$

with λ_i being the eigenvalues of the gyration tensor $Q_{ij} = \frac{1}{N} \sum_{n=1}^N (x_n^i - x_{\text{CM}}^i)(x_n^j - x_{\text{CM}}^j)$, $i, j = 1, \dots, d$, where x_n^j is the j th coordinate of the position vector of the n th monomer of a polymer chain ($n = 1, \dots, N$), and $x_{\text{CM}}^j = \sum_{n=1}^N x_n^j / N$ is the coordinate of the center-of-mass position vector, $\bar{\lambda} \equiv \text{Tr } \mathbf{Q} / d$, and $\hat{\mathbf{Q}} \equiv \mathbf{Q} - \bar{\lambda} \mathbf{I}$ with \mathbf{I} denoting the

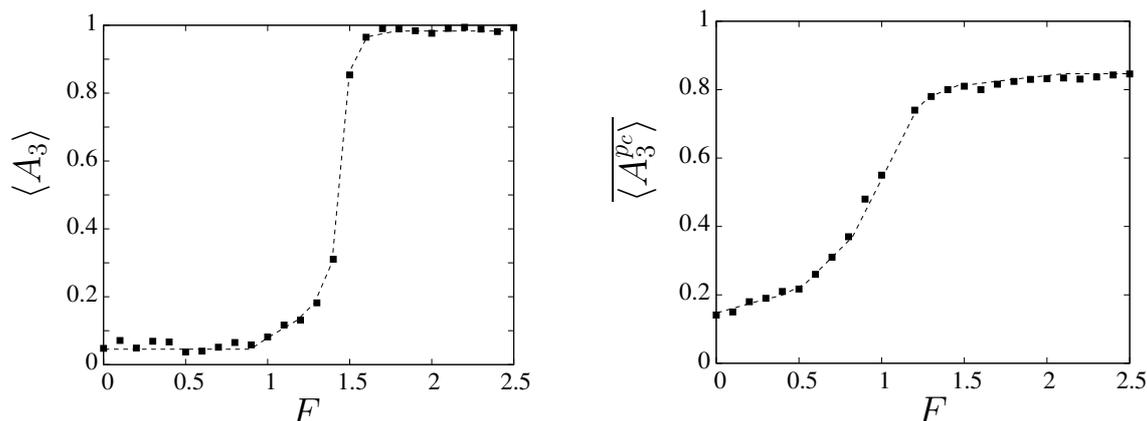


Figure 10.8: Averaged asphericity of an $N = 90$ -step SASAW as function of applied force F in $d = 3$ below the Θ -point. *Left:* Pure lattice ($T = 1.8$). *Right:* Backbone of percolation cluster ($T = 0.2$). Lines are guides to the eyes.

unity matrix. This universal quantity equals zero for a spherical conformation, where all the eigenvalues are equal, and takes a maximum value of one in the case of a rod-like conformation, where all the eigenvalues equal zero except of one. Thus, the inequality $0 \leq A_d \leq 1$ holds. It was realized experimentally [3] that the majority of globular proteins are characterized by $\langle A_d \rangle \approx 0.1$, thus being almost spherical.

A subject of great importance in polymer physics is the understanding of the behaviour of macromolecules in the presence of structural disorder [4]. Biological cells, for instance, can be described as a very crowded environment built of biochemical species that occupy a large fraction of the total volume. In lattice models, such a crowded environment can be described by assigning obstacles to a certain fraction of randomly chosen sites [5]. In this situation one is often interested in the response of polymers to applied tension and stress. Of special interest in biophysics is the stretching of globular polymers below the Θ -point. Applied force not only influences the structural properties of polymers, but also may introduce a new completely stretched state which is otherwise not accessible [6].

Figure 10.8 shows the averaged asphericity of SASAWs, giving information about the internal structure of the polymer conformation under applied force, at a temperature well below the Θ -point for the cases of a pure lattice and the backbone of a percolation cluster modeling the crowded medium [7]. Note that in the absence of force, $\langle A_3 \rangle$ for SASAWs on a pure lattice is very close to zero, whereas in the disordered case, due to the complicated structure of the underlying percolative lattice, globular conformations are more elongated with larger $\langle A_3^{pc} \rangle$ values. At small F , a polymer chain is still in the compact folded state and is just slightly oriented along the force direction. Under increasing force, the polymer chain takes on a conformation similar to the extended (swollen) structure. Note, that completely stretched states, corresponding to $\langle A_d \rangle \approx 1$, can be obtained only in the pure case. In contrast, they are not accessible on the percolative lattices due to the complicated fractal structure of the underlying percolation cluster.

[1] A.Y. Grosberg, A.R. Khokhlov: *Statistical Physics of Macromolecules* (American

- Institute of Physics, New York 1994); C. Vanderzande: *Lattice Models of Polymers* (Cambridge University Press, Cambridge (England) 1998)
- [2] V. Blavatska, W. Janke: *J. Chem. Phys.* **133**, 184903 (2010)
- [3] R.I. Dima, D. Thirumalai: *J. Phys. Chem. B* **108**, 6564 (2004); C. Hyeon et al.: *J. Chem. Phys.* **125**, 194905 (2006); N. Rawat, P. Biswas: *J. Chem. Phys.* **131**, 165104 (2009)
- [4] S. Kumar, M.S. Li: *Phys. Rep.* **486**, 1 (2010)
- [5] V. Blavatska, W. Janke: *Europhys. Lett.* **82**, 66006 (2008); *Phys. Rev. Lett.* **101**, 125701 (2008); *J. Phys. A* **42**, 015001 (2009)
- [6] V. Blavatska, W. Janke: *Phys. Rev. E* **80**, 051805 (2009); in: *Computer Simulations in Condensed Matter Physics XXII*, ed. by D.P. Landau et al., *Physics Procedia* **3**, 1431 (2010)
- [7] V. Blavatska, W. Janke: *Comput. Phys. Commun.* **182**, 1966 (2011)

10.8 Scale-Free Enumeration of Self-Avoiding Walks on Critical Percolation Clusters

N. Fricke, W. Janke

Self-avoiding walks on randomly diluted lattices have attracted much interest over the last decades. They are a basic model for polymers in disordered media and feature universal scaling behaviour with non-trivial exponents [1]. The scaling of the end-to-end distance R and the number of chain conformations Z with the number of steps N is described by the universal exponents ν and γ :

$$\left[\sqrt{\langle R^2 \rangle} \right] \sim N^\nu, \quad [Z] \sim \mu^N N^{\gamma-1}. \quad (10.2)$$

Here μ is the (non-universal) connectivity constant, and the square brackets denote quenched averages over all disorder configurations.

Most interesting is the case at the critical percolation threshold where the fractal dimension of the substrate changes and the disorder covers all length scales. To investigate this problem, researchers have used Monte Carlo simulations, field-theoretical renormalization techniques, as well as exact enumeration. The last method has the benefit of yielding exact results (for single disorder configurations) but is normally limited to very small systems ($N \approx 45$ in 2D [2]) as the computational effort increases exponentially with N .

We found, however, that this exponential complexity can be circumvented through the use of physical ideas: At the percolation threshold, a cluster of occupied sites that spans the whole system is self-similar and just barely connected. It can therefore be decomposed into a hierarchy of nested “blobs”, each of which has only a small number of “children” and few connecting sites to its “parent” (see Fig. 10.9). To determine the different self-avoiding walk conformations through a blob, we only need to enumerate the paths that lie outside of its children and connect them with the paths through the children, which can be counted separately. Starting with the smallest blobs, this procedure can be applied recursively. That way it is possible to enumerate walks of $N = 1000$ steps in a couple of minutes (which otherwise would take over 10^{150} years).

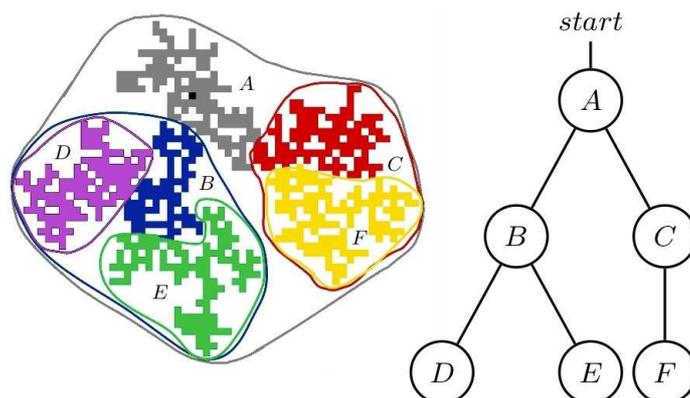


Figure 10.9: Decomposition of a critical percolation cluster and corresponding tree hierarchy. The starting position of the walker is marked in black (in blob A).

Thus we were able to enumerate all self-avoiding walks of 1000 steps on 2×10^5 clusters, allowing us to estimate the scaling exponents with unprecedented accuracy [3]. So far we have implemented the method only in 2D, but the adaptation to three and more dimensions is in progress.

- [1] B. Barat, B.K. Chakrabarti: *Phys. Rep.* **258**, 377 (1995)
- [2] A.R. Singh et al.: *J. Chem. Phys.* **131**, 065103 (2009)
- [3] N. Fricke, W. Janke: *Scale-free enumeration of self-avoiding walks on critical percolation clusters*, Leipzig preprint (2011), submitted to *Europhys. Lett.*

10.9 Two-Dimensional Pinned Flexible Polymers in Hard-Disk Disorder

S. Schöbl, J. Zierenberg, W. Janke

The upcoming interest of physicists in biological systems during the last twenty years has strongly reinforced the interest in polymeric systems. Especially the interest in polymers exposed to disorder has gained great importance as interaction of polymers with their natural environment is a common situation in vivo. This study is concerned with a systematic investigation of pinned polymers located in two-dimensional hard-disk disorder.

The flexible polymer is modeled as a freely jointed chain, consisting of N non-interacting monomers. It can be considered as a random walk with $N - 1$ steps. We investigated this model with the intention to include bending energy between neighboring bonds later on, which describes semiflexible polymers. The disorder is modeled as hard disks that occupy the sites of a square lattice with a certain probability p . The interaction between polymer and disorder is steric, i.e., the monomers are not allowed to sit on the disks. We chose this arrangement in order to be able to control arising subtle structures such as cavities and channels [1]. Exemplary polymer conformations can be seen in Fig.10.10(a).

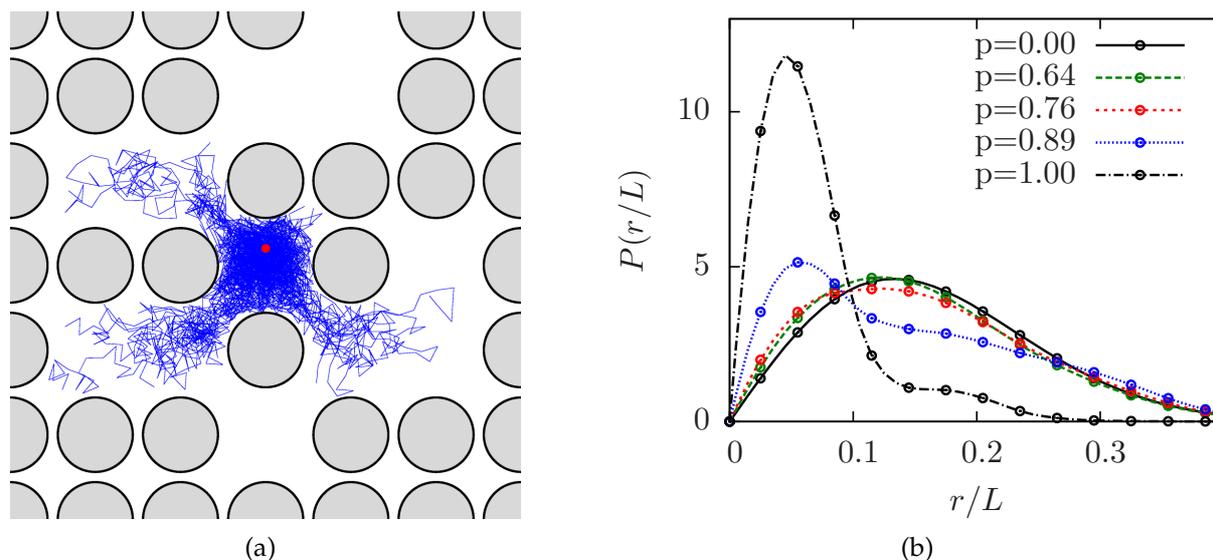


Figure 10.10: (a) Exemplary disorder configuration and typical polymer conformations. (b) The end-to-end distribution function of a flexible polymer with $N = 30$ monomers and bond length b , exposed to hard-disk disorder with different occupation probabilities on a square lattice. The diameter of the disks $\sigma = 4.5b$ is slightly smaller than the lattice constant $a = 5b$.

In a first step, we applied two conceptually different algorithms to the problem addressed here. For one thing, we used an off-lattice chain growth algorithm [2], for another thing we applied the multicanonical Monte Carlo method to the problem.

We considered quenched disorder averages at different occupation probabilities p and were able to show that both algorithms yield the same results within the chosen parameter range (see, e.g., Fig. 10.10(b)). We could clearly approve results from literature [3], namely that high densities strongly influence the extension of flexible polymers, causing a shift in the end-to-end distribution to shorter end-to-end distances. Beyond that, we investigated in detail the effect of small structures such as narrow channels and cavities on the statistical properties of the polymer [1].

[1] S. Schöbl et al.: Phys. Rev. E **84**, 051805 (2011)

[2] T. Garel, H. Orland: J. Phys. A **23**, L621 (1990)

[3] A. Baumgärtner, M. Muthukumar: J. Chem. Phys. **87**, 3082 (1987)

10.10 Development of a Framework Allowing fast Programming of Monte Carlo Simulation of Polymers

M. Marenz, J. Zierenberg, W. Janke

We have started to create an environment for writing fast and efficient Monte Carlo (MC) simulations for arbitrary polymer models. Simulations of such systems yield a better understanding of the behaviour of polymers in specific circumstances [1], or may provide a good initial guess for creating new ones with specific properties [2]. There are a lot of different Molecular Dynamics (MD) programs available, which are capable

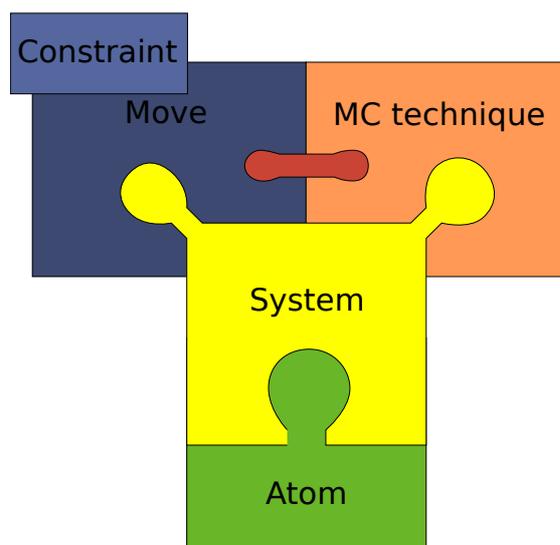


Figure 10.11: The five basic building blocks of the MC simulations framework.

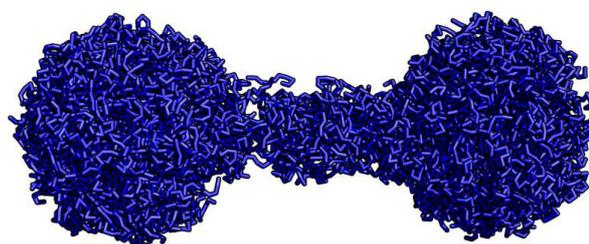


Figure 10.12: Overlay of 1000 steps of one MC simulation of a polymer in a barbell confinement.

of simulating biological or synthetic polymers. However, their abilities to perform MC simulations are rather limited because sophisticated update algorithms are, if at all, implemented only rudimentary. Although MC techniques, in contrast to MD, cannot investigate dynamical properties, they are very convenient for investigating phase transitions and the general character of phase space of arbitrary models in a very efficient manner. The efficiency comes from the broad range of improved MC techniques and the possibility to design a suitable propagation of the system as a Markov process freely.

Unfortunately there exists no widely-used program for MC simulations of polymers. To write a single program which implements all these techniques and possibilities at the same time and still remains efficient is nearly impossible. The alternative, writing a new program from scratch for every demand could be very annoying. That is one reason, why we developed a framework for MC simulations of polymers. The aim of this framework is to provide an environment in the C++ programming language, allowing to perform MC simulations for specific problems in a short time. Another goal of the framework is the expandability. Thus, one can add new methods, potentials, systems and update methods, without adjusting all other parts of the framework. To achieve this goal we divided the problem into single parts, which fit into each other. One can imagine every part as a brick, which can be combined in order to construct a simulation.

There are five basic building blocks: The smallest building blocks are the atoms. The next block is the system, which combines all needed atoms and defines the Hamiltonian of the physical system. On top of the system are the last two main building blocks, the update move and the MC technique. Moves define single updates of the system, propagating from the current state to the next one. Additionally a constraint can be added to every move, in order to simulate a polymer in confinement. An organogram of the simulation framework is sketched in Fig. 10.11.

Until now, we have implemented several MC techniques such as parallel tempering [3], multicanonical [4], Wang-Landau [5] and of course Metropolis Monte Carlo [6]. As

system there are all kinds of linear polymers available, such as simple bead-spring or bead-stick models, with Lennard-Jones, spring, FENE and bending potentials. Adding further pair or bending potentials is extremely simple. We have also implemented confinement constraints such as steric walls, a sphere or a barbell.

As first examples, we are looking at the behaviour of a homopolymer in two different confinements, a polymer inside a sphere and inside a barbell (cf. Fig. 10.12). One important question here is to what extent the confinement modifies the phase transition properties compared to those of a free polymer.

- [1] M. Möddel et al.: Phys. Chem. Chem. Phys. **12**, 11548 (2010); Macromolecules **44**, 9013 (2011)
- [2] M. Bachmann et al.: Angew. Chem. Int. Ed. **49**, 9530 (2010) [Angew. Chem. **122**, 9721 (2010)]
- [3] K. Hukushima, K. Nemoto: J. Phys. Soc. Japan **65**, 1604 (1996)
- [4] B.A. Berg, T. Neuhaus: Phys. Lett. B **267**, 249 (1991); Phys. Rev. Lett. **68**, 9 (1992)
- [5] F. Wang, D. P. Landau: Phys. Rev. Lett. **86**, 2050 (2001); Phys. Rev. E **64**, 056101 (2001)
- [6] W. Janke: Lect. Notes Phys. **739** (Springer, Berlin 2008), pp. 79-140; *Monte Carlo simulations in statistical physics – From basic principles to advanced applications*, Leipzig preprint, invited lecture notes, to appear in: *Order, Disorder and Criticality: Advanced Problems of Phase Transition Theory*, Vol. 3, edited by Y. Holovatch (World Scientific, Singapore 2012), in print

10.11 Stochastic Description of a Binary Frustrated Unit

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Oscillations are an essential feature of processes in biological systems. Biological oscillators can be found in vivo in a multitude of different realizations such as the regulatory glycolytic oscillator, circadian clocks or regulatory genetic circuits. In the description of biological oscillators, two elements are identified to be essential: an inhibitory feedback loop and a source of delay in that loop allowing the oscillating variables to overshoot a steady state [1].

We considered a biological oscillator realized as a simple genetic regulatory circuit [Figs. 10.13(a), (b)] with two populations of proteins A and B, where higher concentration of A *activates* production of A and B while higher concentration of B *inhibits* production of A which, in turn, leads to frustration effects. Oscillations manifest themselves as limit cycles in a Hopf bifurcation with the activated protein production rate α acting as the principal bifurcation parameter [2].

We employed both analytical and numerical methods to analyze the dynamic properties: Treatment of the non-linear master equation using a linear noise approximation, simulation of the stochastic process using a continuous time Monte Carlo method [3]. With those methods we were able to reproduce the limit of the continuous system to check the validity of our extended models. We then focused on the new aspects of the stochastically implemented model, especially for very small systems ($N_{A,B} < 100$):

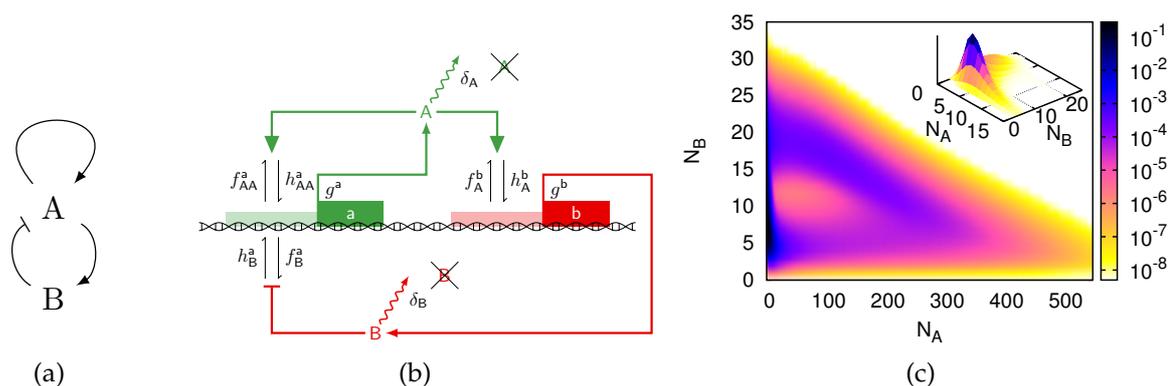


Figure 10.13: (a) Basic motif of the oscillatory genetic circuit. (b) Implementation of the basic motif in a more detailed model with protein production rates controlled by gene states. These in turn are switched through binding of the activator/inhibitor protein to the respective genes promoter regions. (c) Probability density plot from the fixed point regime ($\alpha = 15$, bifurcation points: $\alpha_1 \approx 31.10, \alpha_2 \approx 98.93$), highlighting the shape of oscillatory trajectories.

- 1) Occurrence of oscillations deep in the fixed point regimes [Fig. 10.13(c)]. Fluctuations drive the system away from the fixed point followed by a large excursion along the trajectory of the limit cycle-regime.
- 2) Stabilization of the oscillatory behaviour against parameter changes (i.e. external influences) [4].

- [1] W.O. Friesen, G.D. Block: *Am. J. Physiol.* **246**, R847 (1984)
 [2] P. Kaluza, H. Meyer-Ortmanns: *Chaos* **20**, 043111 (2010)
 [3] D.T. Gillespie: *J. Phys. Chem.* **81**, 2340 (1977)
 [4] A. Garai et al.: *J. Stat. Mech.* P01009 (2012)

10.12 Mass Condensation in Stochastic Transport Models

E. Ehrenpreis, H. Nagel, W. Janke

Generic examples for stochastic mass transport processes are traffic flow, force propagation in granular media, aggregation and fragmentation of clusters, and many others [1]. The transport is classically modeled by probabilities for hopping events from one site to another. Since such processes are usually out-of-equilibrium, it is in general difficult to predict possible stationary states. Still, in some cases it is possible to identify a transition between a liquid-like phase and a phase with a condensate (e.g., a “traffic jam”) that are associated with different stationary states. One speaks of a condensate when a finite fraction M' of constituent particles condenses onto a finite extension W in space, sometimes even onto a single site. This can be observed in the thermodynamic limit where the number of particles M along with the volume N is sent to infinity, with the density $\rho = M/N$ hold fixed. The formation of a condensate is an example for spontaneous symmetry breaking which here, in contrast to equilibrium systems, can happen even in a one-dimensional system.

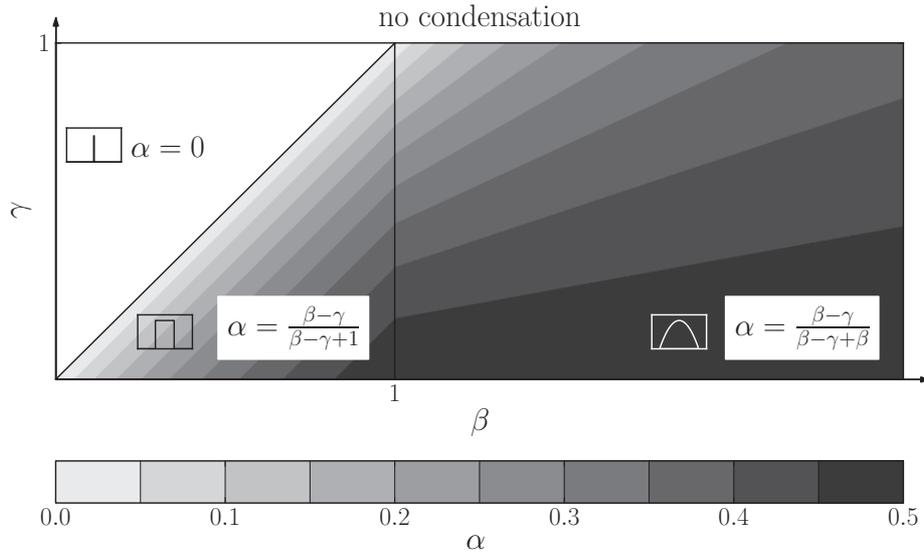


Figure 10.14: Theoretically predicted phase diagram for $K(x) \sim e^{-x^\beta}$ and $p(m) \sim e^{-m^\gamma}$, exhibiting condensed phases with point-like, rectangular and parabolic shapes (from left to right). The predicted value of the exponent α in the scaling law for the condensate extension W with the number M' of condensed particles, $W \simeq M'^\alpha$, is indicated by the gray code.

In previous analytical work [2–4] we concentrated on a class of models with steady states that factorize over the links of arbitrary connected graphs, so-called pair-factorized steady states (PFSS). This property enables at least partially an analytic treatment of the transport properties. In one dimension we could predict the critical mass density at the condensation transition and in particular the condensate shape and its scaling with the system size. The shape of the condensate turned out to be not universal. Rather it can be tuned from “extended” to “point-like” via the competition of local (K) and ultralocal (p) interactions that are implemented in the hopping rates of the stochastic transport process [5]. The resulting phase diagram for the choice $K(x) \propto \exp(-x^\beta)$ and $p(m) \propto \exp(-m^\gamma)$ and the predicted exponent α in the scaling law for the condensate extension, $W \sim M'^\alpha$, are shown in Fig. 10.14.

Since the analytical treatment is based on several approximations, we have performed extensive computer simulations of the hopping events [6]. As a result we find a very nice qualitative agreement of the numerically determined phase diagram with the theoretical prediction given in Fig. 10.14. This is demonstrated in Fig. 10.15 where the measured condensate shapes are displayed in the β - γ plane. By performing the power-law fits of the obtained condensate widths W against the number of constituent particles M' , we also find very good agreement with the predicted values of the exponent α : In most parts of the β - γ plane the agreement is better than 1%.

- [1] M.R. Evans et al.: Phys. Rev. Lett. **97**, 010602 (2006)
- [2] B. Waław et al.: J. Phys. A: Math. Theor. **42**, 315003 (2009)
- [3] B. Waław et al.: Phys. Rev. Lett. **103**, 080602 (2009)
- [4] B. Waław et al.: J. Stat. Mech. P10021 (2009)

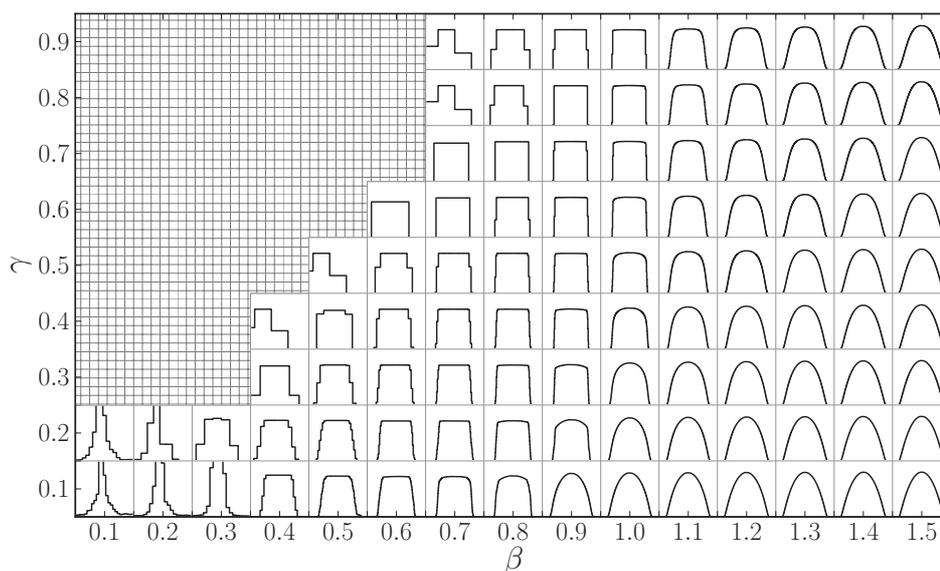


Figure 10.15: Numerically determined characteristic condensate shapes for systems of various β and γ at a condensate volume of about 10^5 masses. The shapes are derived from averages over many measured condensate states. The point-like shapes in the upper left region of the parameter space have not been identified with the present techniques.

[5] B. Waław et al.: J. Phys.: Conf. Ser. **246**, 012011 (2010)

[6] E. Ehrenpreis et al.: Leipzig preprint in preparation

10.13 Mixed Heisenberg Spin Chains: Theory and Quantum Monte Carlo Simulations

R. Bischof, W. Janke

The original Heisenberg model (developed by Heisenberg during his time in Leipzig) and its variants are the basis for understanding quantum magnetism. For instance high-temperature superconducting cuprates can be successfully described as 1D and 2D quantum antiferromagnets at low doping. Depending on the size of the spins and types of coupling mechanisms, the model exhibits a rich variety of zero-temperature quantum critical phenomena. It is well known that uniform chains of half-odd integer spins have no energy gap between the ground state and first excited states (i.e., they are quantum critical), whereas chains with integer spins do show an excitation gap [1]. Moreover by tuning appropriate parameters (such as bond alternation, exchange anisotropy, next-nearest-neighbour interaction, spin-phonon coupling, etc.), spin chains can be driven to or away from criticality.

In this project we consider mixed anisotropic Heisenberg (XXZ) spin chains with bond alternation for which much less is known than for uniform chains. Specifically, our focus is on two different mixed quantum XXZ chains consisting of two different

kinds of spins, $S_a = 1/2$ and $S_b = 1$ or $3/2$, that appear alternately in pairs [2]. In order to investigate their quantum critical properties we employ self-implemented versions of the continuous time loop algorithm [3] and Lanczos exact diagonalization. By successful generalization of recently proposed quantum reweighting methods [4] to improved estimators of the loop algorithm, we have been able to determine the phase diagram in the XY-like region to high precision and could establish a line of continuously varying critical exponents. This strongly suggests that mixed spin chains are in the Gaussian universality class characterized by a central charge of $c = 1$. Furthermore, we could show the presence of logarithmic corrections in the mixed spin models at the SU(2) symmetric isotropic point. These logarithmic corrections influence the scaling and finite-size scaling behaviour on all length scales, which makes the extraction of critical exponents particularly difficult. It is well known that the homogeneous spin chains of $S = 1$ do exhibit such types of corrections [5].

By invoking conformal field theory, we have identified several scaling dimensions that can all be parametrized in terms of one fundamental parameter, a typical sign of the Gaussian universality class. To this end we proposed novel string-like order parameters as a generalization of the disorder parameters of the quantum Ashkin-Teller model. For the $S = 1$ chain our generalization corresponds to the order parameter of the dimerized phase in contrast to the usual string order parameter of the Haldane phase. These new order parameters offer access to scaling dimensions that differ from those of spin operators. As a consequence, the validity of scaling relations can be tested with higher accuracy [7].

Another exotic order parameter is the twist order parameter [6] that is particularly well suited to signal quantum phase transitions between different valence-bond configurations in 1D chains. Despite its potential to accurately locate pseudo-critical points in quantum Monte Carlo simulations, its scaling behaviour has not yet been studied. Our attempts to identify scaling behaviour seem to fail due to the inherently non-local nature of the twist order parameter [7], even though according to [6] a scaling dimension can be assigned.

- [1] F.D.M. Haldane: Phys. Rev. Lett. **50**, 1153 (1983)
- [2] K. Takano: Phys. Rev. Lett. **82**, 5124 (1999); Phys. Rev. B **61**, 8863 (2000); Z. Xu et al.: Phys. Rev. B **67**, 214426 (2003)
- [3] B.B. Beard, U.J. Wiese: Phys. Rev. Lett. **77**, 5130 (1996); H.G. Evertz: Adv. Phys. **52**, 1 (2003)
- [4] M. Troyer et al.: Braz. J. Phys. **34**, 377 (2004)
- [5] C.J. Hamer et al.: Phys. Rev. Lett. **68**, 214408 (2003); T. Papenbrock et al.: Phys. Rev. B **68**, 024416 (2003)
- [6] M. Nakamura, S. Todo: Phys. Rev. Lett. **89**, 077204 (2002)
- [7] R. Bischof, W. Janke: To be published

10.14 Directional Ordering in the Three-Dimensional Compass Model

M.H. Gerlach, W. Janke

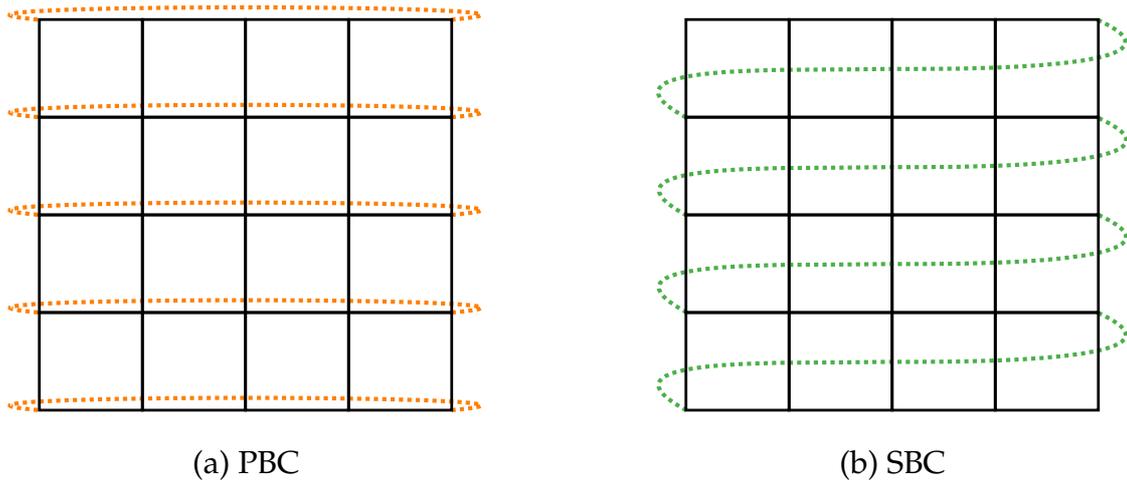


Figure 10.16: Sketch of periodic (PBC) and screw-periodic boundary conditions (SBC) along the x -axis of a two-dimensional lattice. In the SBC picture the link between the lower right and the upper left corner is not shown. Equivalent boundary conditions are applied to the y -direction. Here a screw parameter of $S = 1$ is used.

Both the classical and the quantum version of the compass model have recently attracted much interest in the literature. The reason is its connection to interesting quantum phenomena ranging from orbital order in transition metal compounds to topologically protected qubits [1–3]. In three dimensions the classical model is defined by the Hamiltonian

$$\mathcal{H} = J \sum_{i=1}^N \left(\sigma_i^x \sigma_{i+e_x}^x + \sigma_i^y \sigma_{i+e_y}^y + \sigma_i^z \sigma_{i+e_z}^z \right), \quad (10.3)$$

where $\sigma = (\sigma^x, \sigma^y, \sigma^z)$ are three-dimensional unit spin vectors, e_x , e_y , and e_z are unit vectors in x , y , and z direction, and J is a coupling constant. Although simple looking at first sight, surprisingly little is known about this model in three dimensions. Most studies so far focused on the two-dimensional analogue which still turned out to be rather hard to study numerically. It was shown to possess rich physics ranging from highly degenerate ground states to quantum phase transitions to an exciting thermal phase transition [4, 5].

In recent analyses of high-temperature series expansions of the three-dimensional quantum model (where the classical spins are replaced by Pauli matrices) it was claimed that this model does not exhibit a phase transition at any finite temperature [6]. This motivated us to consider first the three-dimensional classical model and to investigate whether this model exhibits a phase transition [7]. To this end we employed state-of-the-art Monte Carlo computer simulations using Metropolis, cluster, and parallel tempering (PT) techniques. From our previous studies in two dimensions [5] we knew that employing so-called screw-periodic boundary conditions [8] sketched in Fig. 10.16 considerably improves the finite-size scaling behaviour of this model. As a result we obtained convincing numerical evidence for a phase transition of first-order at the temperature $T_0 = 0.098328 \pm 0.000003$. This value is in good agreement with a brief remark in Ref. [9]. The nature of the phase transition can be read off from the histograms

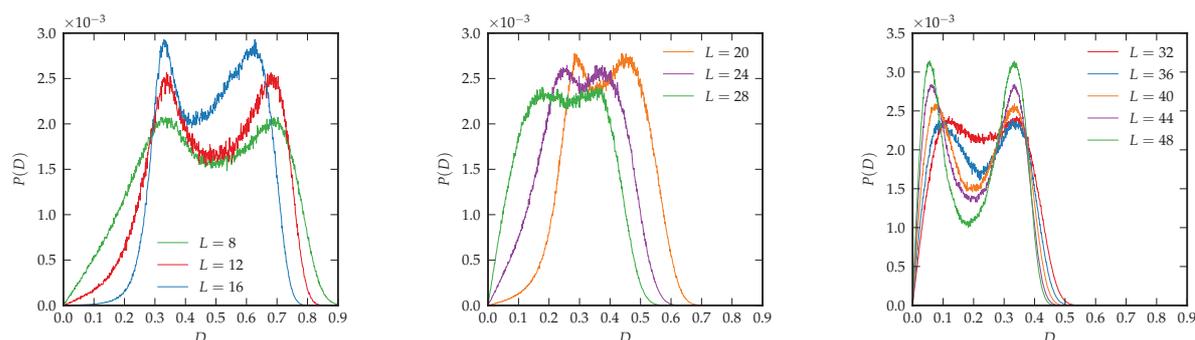


Figure 10.17: Histograms of the directional order parameter D in the three-dimensional compass model with screw-periodic boundary conditions for various lattice sizes L .

of the directional order parameter D of the model in Fig. 10.17 which exhibit for large lattice sizes L a characteristic double-peak structure. Note the nonmonotonic behaviour as function of lattice size: Initially, the double peak becomes *less* pronounced until $L \approx 28 - 32$, and only from then on it becomes more pronounced with further increasing L . By analyzing the ratio of peak maximum to peak minimum, we arrive at a definitely nonzero, albeit small value for associated interface tension, $\sigma_{od} \approx 3 \times 10^{-4}$.

- [1] K.I. Kugel, D.I. Khomskii: Sov. Phys. Usp. **25**, 231 (1982)
- [2] B. Douçot et al.: Phys. Rev. B **71**, 024505 (2005)
- [3] A. Kitaev: Ann. Phys. **321**, 2 (2006)
- [4] S. Wenzel, W. Janke: Phys. Rev. B **78**, 064402 (2008); see also “Publisher’s Note” in Phys. Rev. B **78**, 099902(E) (2008) [Fig. 1 selected for Phys. Rev. B “Kaleidoscope” August 2008]
- [5] S. Wenzel et al.: Phys. Rev. E **81**, 066702 (2010) [arXiv:1002.3508]
- [6] J. Oitmaa, C.J. Hamer: Phys. Rev. B **83**, 094437 (2011)
- [7] M.H. Gerlach, W. Janke: Leipzig preprint in preparation
- [8] E. Bittner et al.: Nucl. Phys. B **820**, 694 (2009)
- [9] S. Wenzel, A.M. Läuchli: Phys. Rev. Lett. **106**, 197201 (2011)

10.15 Multicanonical Analysis of the Goniherdic Ising Model and its Dual

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Heriot-Watt University, Edinburgh, UK

Fluctuating random surfaces are of great interest in condensed matter and high energy physics – and appear in interdisciplinary research on complex networks of membranes and other biological systems, too [1]. One special case is the Goniherdic Ising model that originates from a discrete bosonic string theory. It describes a surface swept out by the string world-sheet as it moves through space-time. The basic properties of such a

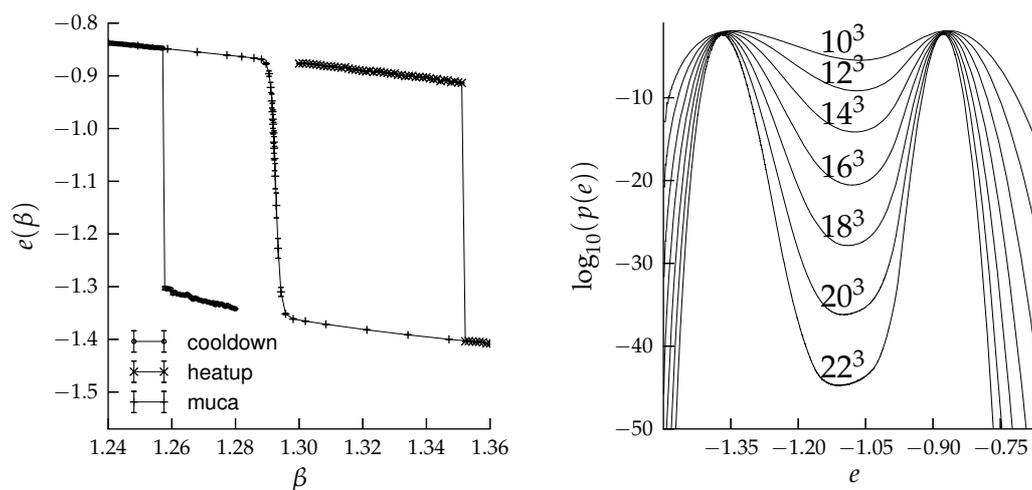


Figure 10.18: *Left:* Hysteresis loop of the dual model and the energy over inverse temperature $\beta = 1/k_B T$ obtained by a multicanonical simulation of the same lattice. The latter is located within the hysteresis loop and should therefore improve any estimates on the transition temperature. *Right:* Energy probability density of the dual model near the phase transition temperature for various lattice sizes. The rare states between the peaks are strongly suppressed but sufficiently sampled by the multicanonical algorithm allowing to extract the interface tension.

surface have been translated into a Hamiltonian of classical Ising spins interacting on a (hyper-)cubic lattice in the 1990s [2, 3]. A $(d - 1)$ -dimensional discretised surface is spanned by plaquettes in the dual lattice that separate spins of opposite sign.

The representation of the surface by classical spins allows the three-dimensional model to be examined by various methods such as mean-field calculations, cluster-variation-Padé-approximation, low-temperature series expansion, the transfer-matrix method and canonical Monte Carlo simulations. All these methods revealed interesting behaviour depending on a control parameter that determines the strength of self-avoidance of the surface. Continuous and discontinuous phase transitions have been found, but the details of the phases are still to be discovered.

In the special case of surfaces that do not suffer an energy penalty upon self-intersection, a first-order phase transition is observed, as well as interesting glassy dynamics upon cooling in simulations [4]. Recently the phase transition has been analysed again using canonical Monte Carlo simulations on dual representations of the model [5–7]. However, the transition temperatures in these studies did not coincide with the original formulation.

We investigated the discontinuous phase transition in the original model and its dual representation with multicanonical simulations that are tailored to overcome slow dynamics in first-order transitions [8]. The transition temperature found by finite-size scaling of the specific heat and Binder’s energy cumulant suggests that the discrepancy in the literature was introduced due to a strong hysteresis effect. The interface tension energetically separating the phases is quite strong and has been measured for both the original model and the dual representation (cf. Fig. 10.18) for the first time.

[1] R. Lipowsky: Nature **349**, 475 (1991)

[2] A. Cappi et al.: Nucl. Phys. B **370**, 659 (1992)

- [3] R.V. Ambartzumian et al.: Phys. Lett. B **275**, 99 (1992)
- [4] D.A. Johnston et al.: in *Rugged Free Energy Landscapes*, ed. W. Janke, *Lecture Notes in Physics*, Vol. **736** (Springer-Verlag, Berlin 2008), pp. 173–199
- [5] D.A. Johnston, R.P.K.C.M. Ranasinghe: J. Phys. A: Math. Theor. **44**, 295004 (2011)
- [6] D.A. Johnston, R.P.K.C.M. Ranasinghe: arXiv:1106.0325 (2011)
- [7] D.A. Johnston, R.P.K.C.M. Ranasinghe: arXiv:1106.4664 (2011)
- [8] M. Müller et al.: Leipzig preprint in preparation

10.16 GPU Computing: Parallel Tempering Simulations of Polymer Statistics

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Graphics processing units (GPUs) have become a very powerful computer platform, in recent years, driven by the professional computer gaming industry. GPUs possess a massively parallel architecture. With the latest release of NVIDIA's convenient programming language CUDA, GPUs have become popular in scientific computing. GPU computing finds its application in many fields, such as astronomy, medicine, time series analysis for financial markets, molecular dynamics simulations, Monte Carlo studies of spin systems, and Quantum Monte Carlo applications [1–3].

We are mainly interested in employing GPU computing for studying the thermodynamical properties of polymer models, both on lattice and off-lattice. The purpose of this project was to investigate whether GPU simulations can be efficiently performed for off-lattice polymer models – without any need of highly sophisticated tricks of implementation. For a straightforward implementation of parallel tempering Monte Carlo simulations [4] of an off-lattice model for elastic polymers we investigated the possible speedup factors on three different GPUs. We tested the two GT200-based GPUs Tesla C1060 (GPU1) and GTX285 (GPU2) with 240 cores and NVIDIA's new generation Fermi-based GTX480 card (GPU3) with 480 cores. As reference CPU system one core of a quadcore Xeon E5620 processor was considered [5, 6].

With the most naive implementation of distributing the replica of the parallel tempering algorithm over the cores, only moderate speed-up factors of about 6 to 9 could be achieved. Having observed that, an improved version was implemented with a parallel calculation of the energy function. This implementation is much faster than the CPU version, when more than 2 replica are simulated. The maximum speed-up factor for the Tesla C1060 card (GPU1) is 68, for the GTX285 card (GPU2) it is 78 and for the Fermi-based GTX480 card (GPU3) even 130, cf. Fig. 10.19. Furthermore it is possible to access multiple graphics cards in a single workstation from one and the same program with no extra effort. Also nodes of established cluster computers can be equipped with GPUs, a combination of the traditional message passing interface (MPI) and CUDA is used in such a scenario. Thus GPUs promise great gains in productivity as well as energy efficiency and are already now on their way to enter the architecture of the next-generation supercomputers [7, 8].

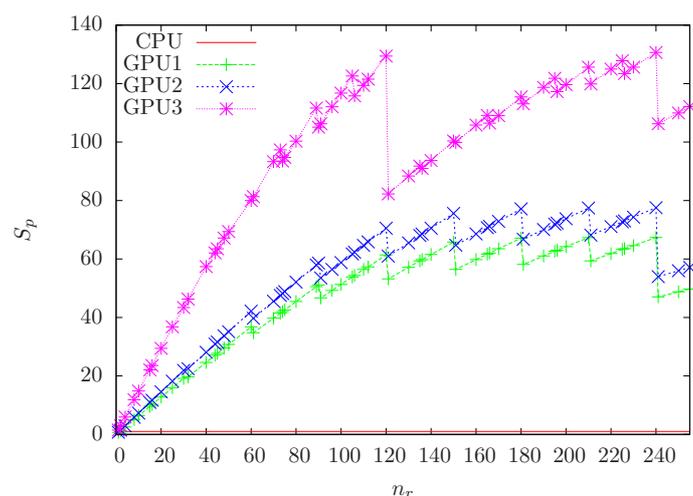


Figure 10.19: Speed-up factor S_p vs number of parallel-tempering replicas n_r for the GPU version with parallelized energy calculation. Drawn lines are only guides to the eye.

- [1] T. Preis et al.: J. Comput. Phys. **228**, 4468 (2009)
- [2] M. Weigel: Comput. Phys. Commun. **182**, 1833 (2011); Phys. Rev. E **84**, 036709 (2011); J. Comput. Phys. **231**, 3064 (2012)
- [3] M. Weigel, T. Yavorskii: Physics Procedia **15**, 92 (2011)
- [4] K. Hukushima, K. Nemoto: J. Phys. Soc. Japan **65**, 1604 (1996)
- [5] J. Gross et al.: Comput. Phys. Commun. **182**, 1638 (2011)
- [6] J. Gross et al.: Physics Procedia **15**, 29 (2011)
- [7] The Top500 List: The 500 most powerful commercially available computer systems, <http://www.top500.org>
- [8] The Green500 List: Environmentally responsible supercomputing, <http://www.green500.org>

10.17 Funding

Graduate School “BuildMoNa”: Leipzig School of Natural Sciences – Building with Molecules and Nano-objects

W. Janke (Principal Investigator)

Deutsche Forschungsgemeinschaft (DFG), Excellence Initiative

Graduate School *Statistical Physics of Complex Systems*

W. Janke (with B. Berche, Nancy)

Deutsch-Französische Hochschule, “Deutsch-Französisches Doktorandenkollegium (DFDK)” with “Co-tutelle de Thèse”, jointly with Nancy Université, France, and Coventry University, UK, as associated partner, Grant No. CDFA-02-07

International Max Planck Research School (IMPRS) *Mathematics in the Sciences*

W. Janke (Scientific Member)

Max Planck Society and Klaus Tschira Foundation

Sonderforschungsbereich/Transregio SFB/TRR 102 *Polymers under Multiple Constraints*:

Restricted and Controlled Molecular Order and Mobility

W. Janke (Principal Investigator, project B04)

Deutsche Forschungsgemeinschaft (DFG)

Forschergruppe 877 From Local Constraints to Macroscopic Transport

W. Janke (Principal Investigator, project P9 in collaboration with K. Kroy)

Deutsche Forschungsgemeinschaft (DFG), Grant No. JA 483/29-1

Host of Prof. Dr. Handan Arkin-Olgar (Ankara University, Turkey), Fellowship for Experienced Researchers

W. Janke

Alexander von Humboldt Foundation

Host of Buket Taşdizen (Ankara University, Turkey), ERASMUS Fellowship

W. Janke

ERASMUS Programme

Dynamik und Statik von Spingläsern

W. Janke

Deutsche Forschungsgemeinschaft (DFG), Grant No. JA 483/22-1

Molecular Conformation Mechanics of Proteins and Polymers

W. Janke

Deutsche Forschungsgemeinschaft (DFG), Grant No. JA 483/24-3

Mass Transport Models on Networks

W. Janke (twin project with H. Meyer-Ortmanns, Jacobs University Bremen)

Deutsche Forschungsgemeinschaft (DFG), Grant No. JA 483/27-1

Grafted and Non-Grafted Polymer Adsorption to (Patterned) Substrates

W. Janke and M. Möddel

NIC Jülich (computer time grant for "JUROPA"), Grant No. hlz17

10.18 Organizational Duties

Wolfhard Janke

- Director, Institute for Theoretical Physics (ITP), Universität Leipzig
- Director, Naturwissenschaftlich-Theoretisches Zentrum (NTZ), Universität Leipzig
- Member of Department Council ("Fakultätsrat"), Faculty for Physics and Earth Sciences, Universität Leipzig
- Member Priority Research Area PbF1 *Molecules and Nano-objects*
- Member Priority Research Area PbF2 *Mathematical Sciences*
- Member of the Steering Committee ("Direktorium") of the Graduate Centre *Mathematics/Computer Science and Natural Sciences*, Research Academy Leipzig
- Spokesperson of the German-French Graduate College *Statistical Physics of Complex Systems*
- Spokesperson of the German-Ukrainian Institute Partnership Leipzig-Lviv of the Alexander von Humboldt Foundation

- Chairperson of the Programme Committee “Scientific Computing” of Forschungszentrum Jülich
- Member of the Scientific-Technical-Council of the Supervisory Board (“Aufsichtsrat”) of the Forschungszentrum Jülich GmbH
- External Member of the Jagiellonian University Graduate School *International Ph.D. Studies in Physics of Complex Systems*, Krakow, Poland
- Specialist Editor, *Computer Physics Communications (CPC)*, Elsevier, Amsterdam, The Netherlands
- Editor “Computational Sciences”, *Lecture Notes of Physics*, Springer, Berlin, Heidelberg, Germany
- Editor “Computational Physics”, *Central European Journal of Physics*, Krakow, Poland
- Member of Editorial Board, *Condens. Matter Phys.*, Lviv, Ukraine
- Permanent Member of the “International Advisory Board”, *Conference of the Middle European Cooperation in Statistical Physics (MECO)*
- Member of the Programme Committee for the *European Conference on Complex Systems 2011 (ECCS’11)*, Vienna, Austria, 12.–16. September 2011
- Member of the Programme Committee for the 4th Conference on *Statistical Physics: Modern Trends and Applications*, Lviv, Ukraine, 03.–06. July 2012
- Co-organizer of the “BuildMoNa” Theory Module *Structure and Mechanics of Foams and Cellular Matter* (with K. Kroy), Universität Leipzig, 22.–23. September 2011
- Organizer of the Workshop *CompPhys11 – 12th International NTZ Workshop on New Developments in Computational Physics*, ITP, Universität Leipzig, 24.–26. November 2011
- Organizer of the Workshop *CompPhys12 – 13th International NTZ Workshop on New Developments in Computational Physics*, ITP, Universität Leipzig, 29. November – 01. December 2012
- External Reviewer for Humboldt-Stiftung (AvH); Deutsche Forschungsgemeinschaft (DFG); Studienstiftung des deutschen Volkes; the Jeffress Memorial Trust, Bank of America, Virginia, USA; “Fond zur Förderung der wissenschaftlichen Forschung (FWF)”, Österreich; “The Royal Society”, Great Britain; The “Engineering and Physical Sciences Research Council (EPSRC)”, Great Britain; The University of Warwick, England, Great Britain; Coventry University, England, Great Britain; CECAM, Lyon, France; National Science Foundation (NSF), USA; Natural Sciences and Engineering Research Council of Canada (NSERC), Canada; Israel Science Foundation, Israel
- Referee for *Physical Review Letters*, *Physical Review B*, *Physical Review E*, *Journal of Chemical Physics*, *Europhysics Letters*, *Physics Letters A*, *Physics Letters B*, *The European Physical Journal B*, *Physica A*, *Proceedings of the Royal Physical Society*, *Journal of Physics A*, *Computer Physics Communications*, *JSTAT*, *New Journal of Physics*, *International Journal of Modern Physics C*

10.19 External Cooperations

Academic

- Institut für Festkörperforschung (IFF-2) and Institute for Advanced Simulation (IAS-

- 2), Forschungszentrum Jülich, Germany
Dr. Michael Bachmann, Jonathan Gross, Dr. Thomas Vogel
- Institute of Physics, Jagiellonian University, Kraków, Poland
Prof. Dr. Piotr Białas, Dr. Leszek Bogacz, Prof. Dr. Zdzisław Burda
 - CEA/Saclay, Service de Physique Théorique, France
Dr. Alain Billoire
 - Institut für Physik, Universität Mainz, Germany
Prof. Dr. Kurt Binder, Dr. Hsiao-Ping Hsu, Andreas Nußbaumer, Prof. Dr. Friderike Schmid, Dr. Martin Weigel
 - Institut für Theoretische Physik, Universität Heidelberg, Germany
Dr. Elmar Bittner
 - Laboratoire de Physique des Matériaux (UMR CNRS No 7556), Nancy Université, France
Prof. Dr. Bertrand Berche, Dr. Christophe Chatelain, Dr. Olivier Collet, Prof. Dr. Malte Henkel, Dr. Dragi Karevski
 - Groupe de Physique des Matériaux (UMR CNRS No 6634), Université de Rouen, France
Dr. Pierre-Emmanuel Berche
 - SUPA, School of Physics and Astronomy, University of Edinburgh, Scotland, UK
Dr. Richard A. Blythe, Prof. Dr. Martin R. Evans, Dr. Bartłomiej Waclaw
 - Istituto Nazionale di Fisica Nucleare, Sezione di Milano-Bicocca, Milano, Italy
Prof. Dr. Pablo Butera
 - Jülich Supercomputing Centre (JSC), Forschungszentrum Jülich, Germany
Prof. Dr. Peter Grassberger, PD Dr. Thomas Neuhaus
 - IAC-1, Universität Stuttgart
Prof. Dr. Rudolf Hilfer, Anjan Prasad Gantapara
 - Complex Systems Division, Department of Theoretical Physics, Lunds Universitet, Lund, Sweden
Prof. Dr. Anders Irbäck, Simon Mitternacht
 - Department of Mathematics and the Maxwell Institute for Mathematical Sciences, Heriot-Watt University, Edinburgh, Scotland, UK
Prof. Dr. Desmond A. Johnston
 - Applied Mathematics Research Centre, Coventry University, England, UK
Dr. Ralph Kenna, PD Dr. Christian von Ferber, Dr. Martin Weigel
 - Inst. für Theoretische Physik, FU Berlin, Germany
Prof. Dr. Hagen Kleinert
 - Max-Planck Institut für Physik komplexer Systeme, Dresden, Germany
Dr. Andreas Läuchli
 - Atominstitut, TU Wien, Austria
Prof. Dr. Harald Markum, Dr. Rainer Pullirsch
 - Jacobs Universität Bremen, Germany
Dr. Ashok Garai, Prof. Dr. Hildegard Meyer-Ortmanns

- Applied Mathematics, Universitat Pompeu Fabra, Barcelona, Spain
Dr. Ramon Villanova
- EPF Lausanne, Switzerland
Dr. Sandro Wenzel
- Department of Engineering of Physics, Ankara University, Turkey
Prof. Dr. Handan Arkın (Olgar), Mustafa Bilsel, Buket Taşdizen
- Dept. of Physics, Hacettepe University, Ankara, Turkey
Prof. Dr. Tarik Çelik, Gökhan Gökoğlu
- Institute for Condensed Matter Physics, National Academy of Sciences, Lviv, Ukraine
Dr. Viktoria Blavatska, Prof. Dr. Yuriy Holovatch
- Yerevan Physics Institute, Yerevan, Armenia
Prof. Dr. David B. Saakian
- Landau Institute for Theoretical Physics, Chernogolovka, Russia
Prof. Dr. Lev N. Shchur
- Banaras Hindu University, Varanasi, India
Prof. Dr. Sanjay Kumar
- Dept. of Physics, Florida State University, Tallahassee, USA
Prof. Dr. Bernd A. Berg
- Dept. of Physics, Michigan Technological University, Houghton, USA
Prof. Dr. Ulrich H.E. Hansmann
- Center for Simulational Physics, The University of Georgia, Athens, USA
Prof. Dr. Michael Bachmann, Jonathan Gross, Prof. Dr. David P. Landau, Dr. Stefan Schnabel, Dr. Thomas Vogel
- Physics Department, Carnegie Mellon University, Pittsburgh, USA
Prof. Dr. Robert H. Swendsen
- Dept. of Physics, Virginia Tech, Blacksburg, USA
Prof. Dr. Michel Pleimling, Prof. Dr. Beate Schmittmann, Prof. Dr. Royce K.P. Zia
- The University of Tokyo, Japan
Prof. Dr. Nobuyasu Ito
- Nagoya University, Japan
Tetsuro Nagai, Prof. Dr. Yuko Okamoto
- Laboratory of Statistical and Computational Physics, Institute of Physics, Academia Sinica, Nankang, Taipei, Taiwan
Prof. Dr. Chin-Kun Hu
- Zhejiang Institute of Modern Physics, Zhejiang University, Hangzhou, P.R. China
Prof. Dr. He-Ping Ying, Prof. Dr. Bo Zheng

10.20 Publications

Journals

E. Bittner, W. Janke: *Parallel-Tempering Cluster Algorithm for Computer Simulations of Critical Phenomena*, Phys. Rev. E **84**, 036701-1–4 (2011)

V. Blavatska, W. Janke: *Θ -Polymers in Crowded Media under Stretching Force*, Comput. Phys. Commun. **182**, 1966–1969 (2011)

J. Gross, W. Janke, M. Bachmann: *Massively Parallelized Replica-Exchange Simulations of Polymers on GPUs*, Comput. Phys. Commun. **182**, 1638–1644 (2011)

J. Gross, W. Janke, M. Bachmann: *A GPU Approach to Parallel Replica-Exchange Polymer Simulations*, in *Computer Simulation Studies in Condensed-Matter Physics XXIV*, eds. D.P. Landau, S.P. Lewis, H.-B. Schüttler, Physics Procedia **15**, 29–32 (2011)

W. Janke, T. Neuhaus, A.M.J. Schakel: *Worms Exploring Geometrical Features of Phase Transitions*, in *Computer Simulation Studies in Condensed-Matter Physics XXIV*, eds. D.P. Landau, S.P. Lewis, H.-B. Schüttler, Physics Procedia **15**, 54–58 (2011)

C. Junghans, W. Janke, M. Bachmann: *Hierarchies in Nucleation Transitions*, Comput. Phys. Commun. **182**, 1937–1940 (2011)

S. Karalus, W. Janke, M. Bachmann: *Thermodynamics of Polymer Adsorption to a Flexible Membrane*, Phys. Rev. E **84**, 031803-1–12 (2011)

M. Möddel, W. Janke, M. Bachmann: *Adsorption of Finite Polymers in Different Thermodynamical Ensembles*, Comput. Phys. Commun. **182**, 1961–1965 (2011)

M. Möddel, W. Janke, M. Bachmann: *Comparison of the Adsorption Transition for Grafted and Non-Grafted Polymers*, Macromolecules **44**, 9013–9019 (2011)

S. Schnabel, W. Janke, M. Bachmann: *Advanced Multicanonical Monte Carlo Methods for Efficient Simulations of Nucleation Processes of Polymers*, J. Comput. Phys. **230**, 4454–4465 (2011)

S. Schöbl, J. Zierenberg, W. Janke: *Simulating Flexible Polymers in a Potential of Randomly Distributed Hard Disks*, Phys. Rev. E **84**, 051805-1–8 (2011)

Books

in press

H. Arkin, W. Janke: *Structural Behavior of a Polymer Chain Inside an Attractive Sphere*, Phys. Rev. E **85**, 051802-1–9 (2012)

M. Bilsel, B. Taşdizen, H. Arkin, W. Janke: *Effects of Confinement on the Thermodynamics of a Model Protein*, to appear in Proceedings of the NIC Workshop *From Computational Biophysics to Systems Biology 2011*, Jülich, 20–22 July 2011, John von Neumann Institute for Computing, Forschungszentrum Jülich, IAS Series, in print (2012)

V. Blavatska, W. Janke: *Polymer Adsorption on a Fractal Substrate: Numerical Study*, J. Chem. Phys. **136**, 104907-1–8 (2012)

V. Blavatska, W. Janke: *Conformational Properties of Polymers Near a Fractal Surface*, in *Computer Simulation Studies in Condensed-Matter Physics XXV*, eds. D.P. Landau, S.P. Lewis, H.-B. Schüttler, to appear in Physics Procedia (2012), in print

N. Fricke, W. Janke: *Exact Enumeration of Self-Avoiding Walks on Percolation Clusters*, in *Computer Simulation Studies in Condensed-Matter Physics XXV*, eds. D.P. Landau, S.P. Lewis, H.-B. Schüttler, to appear in Physics Procedia (2012), in print

A. Garai, B. Waclaw, H. Nagel, H. Meyer-Ortmanns: *Stochastic Description of a Bistable Frustrated Unit*, J. Stat. Mech. P01009 (2012)

W. Janke: *Monte Carlo Simulations in Statistical Physics – From Basic Principles to Advanced Applications*, invited lecture notes, to appear in *Order, Disorder and Criticality: Advanced Problems of Phase Transition Theory*, Vol. 3, ed. Y. Holovatch (World Scientific, Singapore 2012), in print

M. Möddel, M. Bachmann, W. Janke: *Grafted versus Non-Grafted Polymer Adsorption*, in *NIC Symposium 2012, Proceedings*, eds. K. Binder, G. Münster, M. Kremer, John von Neumann Institute for Computing, Forschungszentrum Jülich, NIC Series, Vol. **45** (2012), pp. 277–284

Talks

H. Arkin: *Simulations of Biological Molecules*, SFG FOR877 Kick-Off Meeting, Universität Leipzig, 24. June 2011

N. Fricke: *A Numerical Study of Self-Avoiding Walks (SAWs) on Disordered Two-Dimensional Lattices*, Spring Meeting of the German Physical Society, Dresden, 18. March 2011

N. Fricke: *Numerical Treatment of Self-Avoiding Walks on Disordered Lattices*, Seminar of the cdfa-dfdk, Nancy, France, 14. June 2011

N. Fricke: *Exact Enumeration of Self-Avoiding Walks on Percolation Clusters*, Applied Mathematics Seminar, Coventry University, UK, 26. October 2011

N. Fricke: *Scale-Free Enumeration of Self-Avoiding Walks on Critical Percolation Clusters*, Seminar of the cdfa-dfdk, Leipzig, 15. December 2011

W. Janke: *The Ising Model in Statistical Physics II*, IMPRS Ringvorlesung “Discrete Structures in Physics”, International Max Planck Research School, Max-Planck-Institut für Mathematik in den Naturwissenschaften, Leipzig, 04. January 2011

W. Janke: *The Ising Model in Statistical Physics III*, IMPRS Ringvorlesung “Discrete Structures in Physics”, International Max Planck Research School, Max-Planck-Institut für Mathematik in den Naturwissenschaften, Leipzig, 11. January 2011

W. Janke: *Worms Exploring Geometrical Features of Phase Transitions*, 24th CSP Workshop on Recent Developments in Computer Simulation Studies in Condensed Matter Physics, The University of Georgia, Athens, USA, 21.–25. February 2011

W. Janke: *Monte Carlo Simulations in Multicanonical Ensembles*, invited talk, 2nd Stellenbosch Workshop on Statistical Physics, NITheP, Stellenbosch, South Africa, 07.–18. March 2011

W. Janke: *Thermodynamics of Polymer Statistics: Perspectives from Three Statistical Ensembles*, invited talk, 2nd Stellenbosch Workshop on Statistical Physics, NITheP, Stellenbosch, South Africa, 07.–18. March 2011

W. Janke: *Worms Exploring Geometrical Features of Phase Transitions*, 36th Conference of the Middle European Cooperation in Statistical Physics MECO36, Institute for Condensed Matter Physics, Lviv, Ukraine, 05.–07. April 2011

M. Marenz: *Worm Algorithm – Simulating Spin Systems via Path Representation*, Seminar of the cdfa-dfdk, Nancy, France, 18. October 2011

M. Möddel: *Effects of Polymer Grafting on the Thermodynamic Equilibrium Behavior of Single Polymer Adsorption*, Spring Meeting of the German Physical Society, Dresden, 16. March 2011

M. Möddel: *Some Aspects of the Thermodynamic Equilibrium Behaviour of a Finite Single Polymer Near an Attractive Substrate*, research seminar, Applied Mathematics Research Centre, Coventry University, Coventry, England, 23. May 2011

H. Nagel: *Stochastic Description of a Bistable Frustrated Unit*, Seminar of the Applied Mathematics Research Centre, Coventry University, 12. October 2011

J. Zierenberg: *Simulating Semiflexible Polymers in Hard Disc Background Potentials*, Seminar of the cdfa-dfdk, Nancy, France, 25. October 2011

Posters

M. Bilsel, B. Taşdizen, H. Arkın, W. Janke: *Effects of Confinement on the Thermodynamics of a Model Protein*, Conference From Computational Biophysics to System Biology 2011, NIC, Forschungszentrum Jülich, 20.–22. July 2011

R. Bischof, W. Janke: *Gaußsche Universalitätsklasse in gemischten Quantenspinketten*, RAL-Evaluation, Universität Leipzig, 10.–19. October 2011

R. Bischof, W. Janke: *Gaussian Universality Class in Mixed Quantum Spin Chains*, 12th International NTZ-Workshop on New Developments in Computational Physics – CompPhys11, Universität Leipzig, 24.–26. November 2011

N. Fricke, W. Janke: *How to count 10^{100} Self-Avoiding Walks on a Critical Percolation Cluster*, Spring Meeting of the German Physical Society, Dresden, 13.–18. March 2011

N. Fricke, W. Janke: *A new Technique for Complete Enumeration of Self-Avoiding Walks on Percolation Clusters*, 36th Conference of the Middle European Cooperation in Statistical Physics *MECO36*, Institute for Condensed Matter Physics, Lviv, Ukraine, 05.–07. April 2011

N. Fricke, W. Janke: *Scale-Free Enumeration of Self-Avoiding Walks on Critical Percolation Clusters*, 12th International NTZ-Workshop on New Developments in Computational Physics – *CompPhys11*, Universität Leipzig, 24.–26. November 2011

M. Marenz, W. Janke: *Worm Algorithm in Ordered and Disordered Media*, Spring Meeting of the German Physical Society, Dresden, 13.–18. March 2011

M. Marenz, W. Janke: *Worm Algorithm in Ordered and Disordered Media*, Mainz Materials Simulation Days, Universität Mainz, 25.–27. May 2011

M. Marenz, W. Janke: *Worm Algorithm in Ordered and Disordered Media*, CECAM Jülich Summer School, Forschungszentrum Jülich, 12.–16. September 2011

M. Möddel, M. Bachmann, W. Janke: *Comparison of Grafted and Non-Grafted Polymer Adsorption in Different Ensembles*, 4th Scientific Symposium of the Graduate School *BuildMoNa*, Universität Leipzig, 21. March 2011

M. Möddel, M. Bachmann, W. Janke: *Comparison of Grafted and Non-Grafted Polymer Adsorption in Different Ensembles*, 12th International NTZ-Workshop on New Developments in Computational Physics – *CompPhys11*, Universität Leipzig, 24.–26. November 2011

H. Nagel, B. Waclaw, W. Janke: *Time Scale of Mass Condensation in Stochastic Transport with Pair Factorized Steady States*, Spring Meeting of the German Physical Society, Dresden, 13.–18. March 2011

S. Schöbl, K. Kroy, W. Janke: *Broadscale Examination of the Influence of Disorder on Semiflexible Polymers*, 4th Scientific Symposium of the Graduate School *BuildMoNa*, Universität Leipzig, 21. March 2011

J. Zierenberg, B.A. Berg, W. Janke: *Structure of the Tip4p Water Model in the Ice I_h Phase*, Spring Meeting of the German Physical Society, Dresden, 13.–18. March 2011

J. Zierenberg, B.A. Berg, W. Janke: *Structure of the Tip4p Water Model in the Ice I_h Phase*, Mainz Materials Simulation Days, Universität Mainz, 25.–27. May 2011

J. Zierenberg, B.A. Berg, W. Janke: *All-Atom Simulations of Tip4p Water on Graphics Cards using OpenGL*, International Symposium *Computer Simulations on GPU*, Universität Mainz, 30. May – 01. June 2011

J. Zierenberg, B.A. Berg, W. Janke: *Structure of the Tip4p Water Model in the Ice I_h Phase*, CECAM Jülich Summer School, Forschungszentrum Jülich, 12.–16. September 2011

10.21 Graduations

Diploma

- Marco Müller
Multicanonical Analysis of the Gonihedric Ising Model and its Dual
01. November 2011

10.22 Guests

- Dr. Stefan Schnabel
University of Georgia, Athens, USA
01.–10. January 2011
- Dr. Bartłomiej Waclaw
University of Edinburgh, UK
NTZ Colloquium/FOR877 Seminar
A Dynamical Phase Transition in a Model for Evolution with Migration
26.–28. January 2011
- Prof. Dr. Yuko Okamoto
Nagoya University, Japan
NTZ Colloquium
Biomolecular Simulations by Efficient Conformational Sampling Techniques
04.–06. May 2011
- Prof. Dr. Royce P.K. Zia
Virginia Tech, Blacksburg, USA
NTZ Colloquium/FOR877 Seminar
Modeling Translation by Totally Asymmetric Simple Exclusion Processes (TASEP)
07. July 2011
- Dr. Christoph Junghans
MPI für Polymerforschung, Mainz, Germany
DFH-UFA Seminar
Locality Analysis via Adaptive Resolution Simulations
11.–13. July 2011
- Dr. Ashok Garai
Jacobs University, Bremen, Germany
DFH-UFA Seminar
Stochastic Simulations of a Bistable Frustrated Unit
12.–14. July 2011
- Jeremi Ochab
Jagiellonian University, Krakow, Poland
Epidemics on Networks
01. August – 31. October 2011
- Dr. Viktoria Blavatska
Institute for Condensed Matter Physics, Lviv, Ukraine

Humboldt Fellow/FOR877 guest
NTZ Colloquium/FOR877 Seminar
Numerical Study of Polymer Adsorption on Fractal Substrates
01. October – 30. November 2011

- Prof. Dr. Robert H. Swendsen
Carnegie Mellon University, Pittsburgh, USA
NTZ Colloquium/DFH-UFA Seminar
The Entropy Wars
23.–29. October 2011
- Prof. Dr. Robert H. Swendsen
Carnegie Mellon University, Pittsburgh, USA
NTZ Colloquium
How the Maximum Step Size in Monte Carlo Simulations Should be Adjusted
20.–26. November 2011
- Pádraig Mac Carron
Applied Mathematics Research Centre, Coventry University, UK
Mythological Networks
22.–28. November 2011
- Prof. Dr. Alexander Hartmann
Universität Oldenburg, Germany
Random-Field Ising Magnet with Correlated Disorder
23.–25. November 2011
- Prof. Dr. Heiko Rieger
Saarland University, Saarbrücken, Germany
Strong Roughening of Spontaneous Imbibition Fronts
23.–25. November 2011
- Prof. Dr. Antun Balaz
Scientific Computing Laboratory, Institute of Physics, University of Belgrade, Serbia
Numerical Simulations of Faraday Waves in Binary Bose-Einstein Condensates
23.–26. November 2011
- Hsiao-Ping Hsu
Universität Mainz, Germany
Structure and Scaling Analysis of Stretched Semiflexible Polymer Chains
23.–26. November 2011
- Prof. Dr. Malte Henkel
Nancy Université, France
Logarithmic Extensions of Local Scale Invariance
23.–27. November 2011
- Prof. Dr. Ferenc Iglói
Institute of Theoretical Physics, Research Institute for Solid State Physics and Optics,
Budapest, Hungary
Quantum Relaxation After a Quench in Systems with Boundaries
23.–27. November 2011

- Prof. Dr. Desmond A. Johnston
Heriot-Watt University, Edinburgh, UK
Gonihedric Ising Models: Order Parameter(s) and Dual(s)
23.–27. November 2011
- Tetsuro Nagai
Nagoya University, Japan
Application of Two-Dimensional Simulated Tempering (ST) to the Two-Dimensional Ising Model
23.–27. November 2011
- Jeremi Ochab
Jagiellonian University, Krakow, Poland
Pair-Factorised Steady State Model Exhibits a Condensate's Growth on Monolayers
23.–27. November 2011
- Prof. Dr. Yuko Okamoto
Nagoya University, Japan
Generalized-Ensemble Simulations of Spin Models and Biomolecular Systems
23.–27. November 2011
- Dr. Sergio Perez-Gaviro
Institute for Biocomputation and Physics of Complex Systems (BIFI), University of Zaragoza, Spain
Anisotropy Impact in the 3D Heisenberg Spin-Glass Model
23.–27. November 2011
- Prof. Dr. Mark Taylor
Hiram College, Hiram, OH, USA
Partition Function Zeros and Phase Transitions of a Polymer Chain
23.–27. November 2011
- Karol Trojanowski
Jagiellonian University, Krakow, Poland
Resonance and Pattern Formation in the Kuramoto Model with Manhattan Delay
23.–27. November 2011
- Marcin Zagórski
Jagiellonian University, Krakow, Poland
Motifs Emerge from Function in Model Gene Regulatory Networks
23.–27. November 2011
- PD Dr. Thomas Neuhaus
Jülich Supercomputing Centre, Forschungszentrum Jülich, Germany
NTZ Colloquium/DFH-UFA Seminar
Numerical Study of Quantum Annealing for the Hardest Case of 2SAT and 3SAT
23. November – 03. December 2011
- Dr. Elmar Bittner
Universität Heidelberg, Germany
Parallel-Tempering Cluster Algorithm for Computer Simulations of Critical Phenomena
24.–28. November 2011

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Precision Calculation of Spin-Spin Correlators in the Ising Model via Worm Updates
25. November 2011
- Buket Taşdizen
Ankara University, Turkey
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